



**Barcelona  
Supercomputing  
Center**  
*Centro Nacional de Supercomputación*



# Atmospheric composition research, modeling and services at BSC

**Carlos Pérez García-Pando**

**María Teresa Pay**

Atmospheric Composition group

**Albert Soret**

Earth System Services group

13/06/2017

ISGlobal Seminar

- Created in 2005; ~500 employees
- Research, develop and manage information technology
- Facilitate scientific progress and its application in society



## Earth Science Department

- Atmospheric composition
- Climate prediction
- Computational Earth Sciences
- Earth System Services





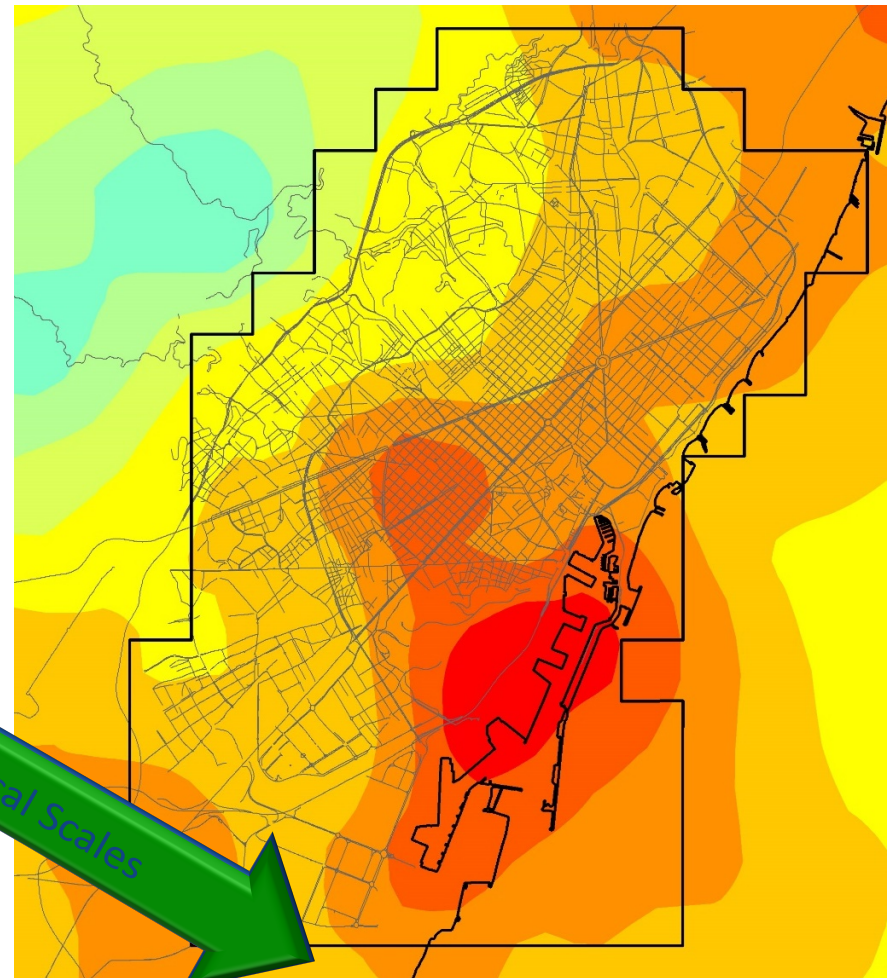
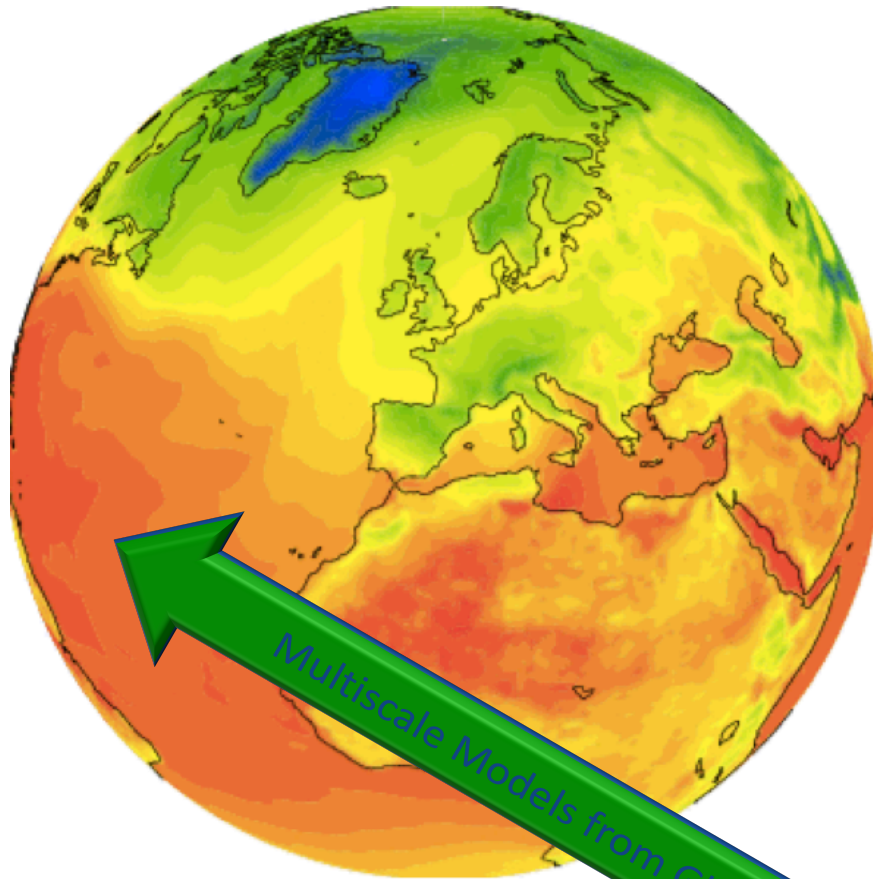
- Atmospheric Composition (AC) group aims at better understanding and predicting the spatiotemporal variations of atmospheric pollutants along with their effects upon air quality, weather and climate.
- Earth System Services (ESS) group facilitates technology transfer of state-of-the-art research from local, national to international levels.

*Performs applied research to demonstrate the ongoing value of climate and atmospheric composition services and advance sustainable development in sectors such as renewable energy, urban development, insurance, agriculture, water management or health.*

- Development of the in-house **MONARCH**, an online **multiscale non-hydrostatic chemical weather prediction system** that can be run either globally or regionally.
- Development of the in-house **multiscale emission model HERMES**
- **Model evaluation** including data from satellites, and lidar, Sun-photometer and in-situ networks, both for gaseous and aerosol species, covering multiple time-scales.
- Development of an **ensemble-based data assimilation** techniques using data from satellites and ground-based observations.
- **Air quality in urban areas**: enhancing modeling approaches, emissions, source attribution and impacts
- **Understanding aerosol processes and effects**, with emphasis on **mineral dust**
- Research backbone of in-house and external forecasting activities:
  - **WMO Sand and Dust Storm Warning Advisory and Assessment System** Regional Center (WMO SDS-WAS RC) for Northern Africa, Middle East and Europe.
  - International Cooperative for Aerosol Prediction (**ICAP**).
  - **CALIOPE** air quality system (“CALIdad del aire Operacional Para España”), which provides high-resolution air quality forecasts over Europe.



## Multi-scale models from global to local scales



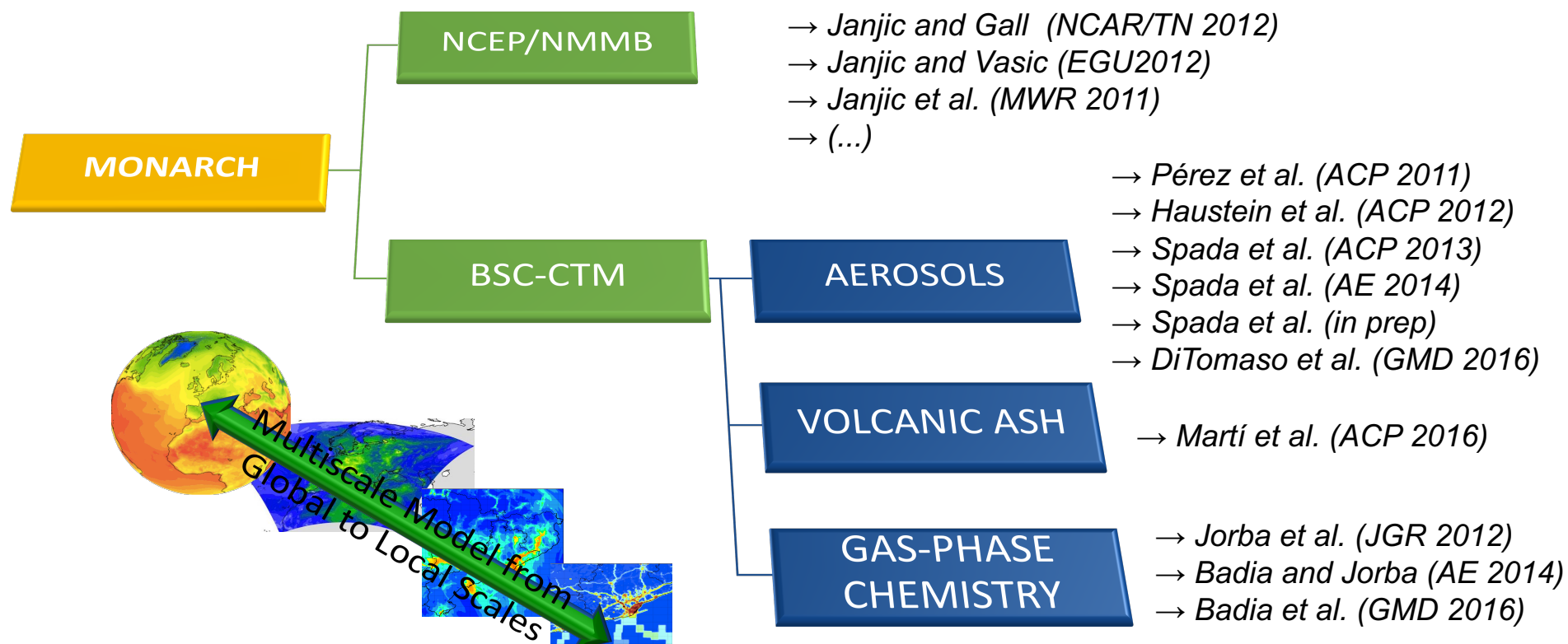
Multiscale Models from Global to Local Scales

**Multiscale:** global to regional scales allowed (nesting capabilities)

**Non-hydrostatic** dynamical core: single digit kilometre resolution allowed

**On-line** coupling: weather-chemistry feedback processes allowed

**Ensemble-based data assimilation** system for aerosols

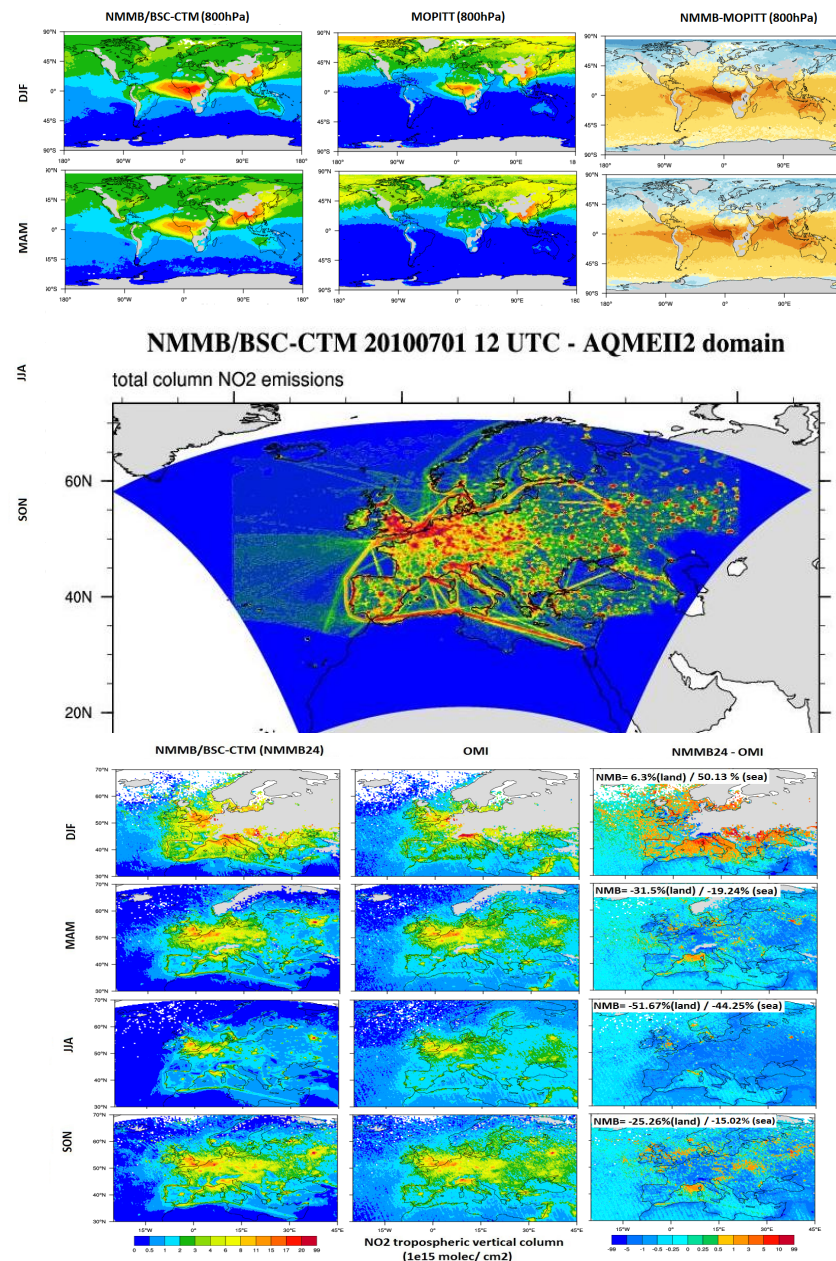




## CURRENT FORECASTING – DEVELOPED/AVAILABLE – UNDER DEVELOPMENT - PLANNED

DOMAIN	GLOBAL (ICAP)	REGIONAL North Africa, Middle East and Europe (SDS-WAS)	REGIONAL Europe/Iberian Peninsula/Urban Areas (CALIOPE)
Model	MONARCH	MONARCH	CMAQ (DREAM for dust) <b>MONARCH</b>
Status	QO	O	O
Meteorology	Inline: NMMB	Inline: NMMB	Offline: WRF-ARW <b>Inline: NMMB nesting</b>
Resolution	1.4x1 deg <b>0.7x0.5 deg</b>	0.1x0.1 deg <b>0.03x0.03 deg</b>	0.1x0.1 / 0.04x0.04 / 0.01 x0.01
levels	24 <b>48</b>	40 <b>60-70</b>	30 <b>60-70</b>
DA	<b>LETKF</b>	<b>LETKF</b>	NA <b>LETKF</b>
Assimilated Obs	<b>MODIS DT+DB (DU)</b> <b>MODIS DT+DB (ALL)</b>	<b>MODIS DT+DB (DU)</b>	NA <b>MODIS DT+DB (ALL)</b>
Aerosol Species	DU, SS, <b>BC</b> , <b>POA</b> , <b>SOA bio</b> , <b>SOA anthro</b> , <b>SU</b> , <b>NI</b>	DU	CMAQ (AERO5) <b>MONARCH aerosols</b>
Gas phase chemistry	<b>CBM-IV</b> <b>CB05</b>		<b>CB05</b> <b>CB05</b>
Emissions	<b>HERMES 3.0 (HTAP v2)</b>		EMEP, MEGAN / HERMES, MEGAN/ HERMES MEGAN
Bio. Burn. Emissions	<b>GFAS</b> <b>NRT</b>		NA <b>NRT</b>

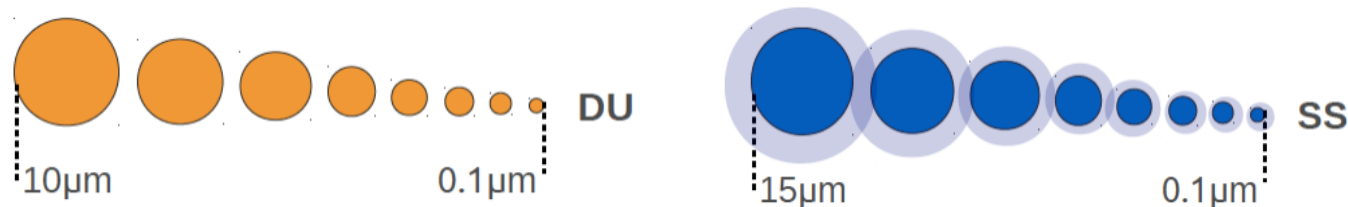
- OH, O<sub>3</sub>, HO<sub>2</sub>: for aerosol calculations we can use **online** gas-phase simulations or **off-line climatologies**
- **Carbon-bond CBM-IV and CB05** mechanisms implemented (Gery et al., 1989; Yarwood, 2005)
- Coupled with **Fast-J photolysis scheme** (Wild et al., 2000)
- Mechanism implemented through **KPP kinetic pre-procesor** (Damian et al., 2002)
- Implemented an **EBI solver for CB05** as in CMAQ. Includes 51 chemical species and 156 reactions. Working version and thoroughly tested.
- **Stratospheric ozone**: linear model Cariolle and Teyssèdre (2007) or Monge-Sanz et al. (2011)





## Sectional

dust (DU)  
sea-salt (SS)



## Bulk

Black Carbon (BC)



Organic Aerosols (OA)

Primary Organic Aerosols (POA)

Secondary organic aerosols (SOA)

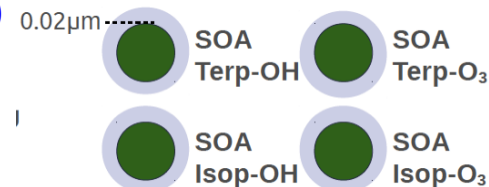
4 gaseous tracers (OH, O<sub>3</sub>, TERP, ISOP). Online emission (MEGAN)

4 aerosol-phase hydrophilic tracers

2-product scheme of Tsigaridis and Kanakidou (2007)

Oxidation by OH and O<sub>3</sub> and gas-particle partitioning

Anthropogenic SOA from Toluene and Xylene under development



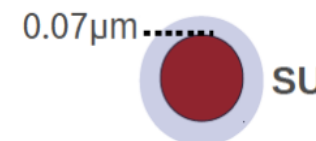
Sulfate (SU):

4 additional prognostic tracers (SO<sub>2</sub>, DMS, H<sub>2</sub>O<sub>2</sub>, H<sub>2</sub>SO<sub>4</sub>)

3 online or climatological oxidants (OH, O<sub>3</sub>, HO<sub>2</sub>)

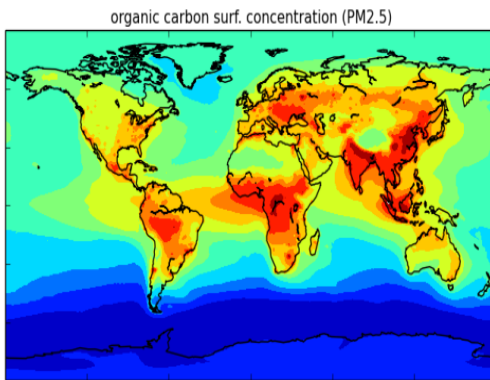
gas-phase oxidation of SO<sub>2</sub>, DMS and H<sub>2</sub>O<sub>2</sub> by OH

aqueous-phase oxidation by H<sub>2</sub>O<sub>2</sub> and O<sub>3</sub>

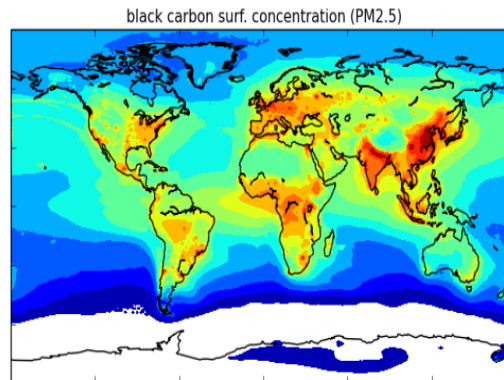


Nitrate (NO<sub>3</sub>) and Ammonium (NH<sub>4</sub>): as calculated by EQSAM  
thermodynamic equilibrium model but not evaluated yet

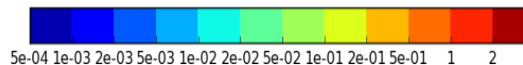
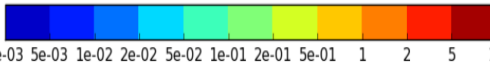
- **Dry deposition:** aerodynamic and surface resistance (Zhang et al., 2001)
- **Gravitational settling:** Stokes approximation, Cunningham correction factor. Both implicit and explicit upwind schemes available.
- **In-cloud and below cloud scavenging** from grid-scale (Ferrier Microphys.) and sub-grid scale (BMJ) clouds
- Below cloud scavenging (directional interception, inertial impaction and Brownian diffusion)
- Vertical **convective mixing** follows the BMJ adjustment scheme (instead of a mass flux scheme)
- Radiation: **RRTM** SW/LW **aerosol radiative feedback**



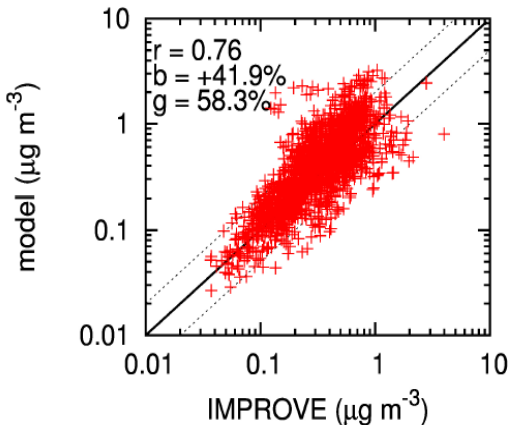
annual average ( $\mu\text{g m}^{-3}$ ); interannual mean over 2002-2006



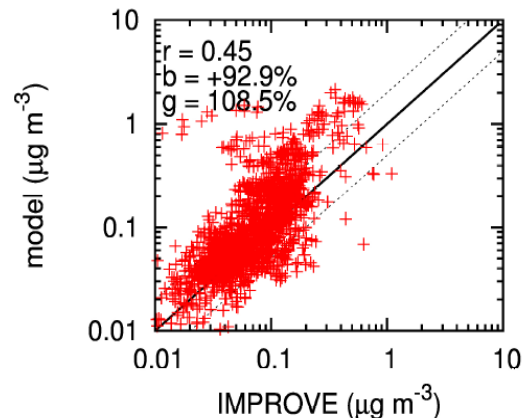
annual average ( $\mu\text{g m}^{-3}$ ); interannual mean over 2002-2006



organic carbon PM2.5 (US)



black carbon PM2.5 (US)

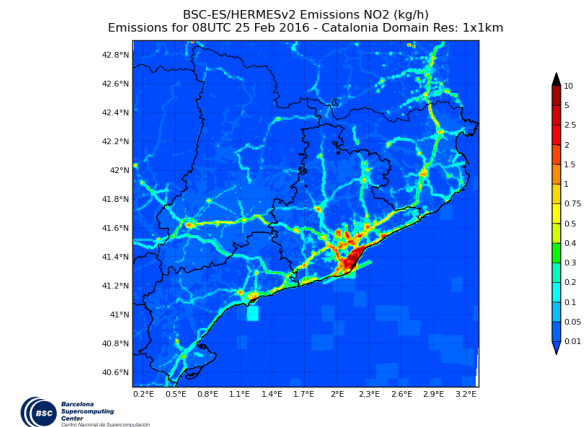
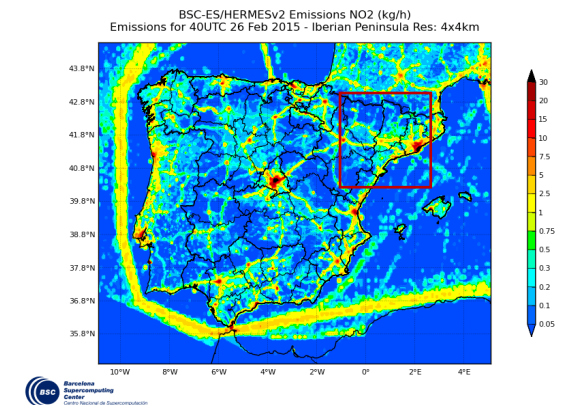
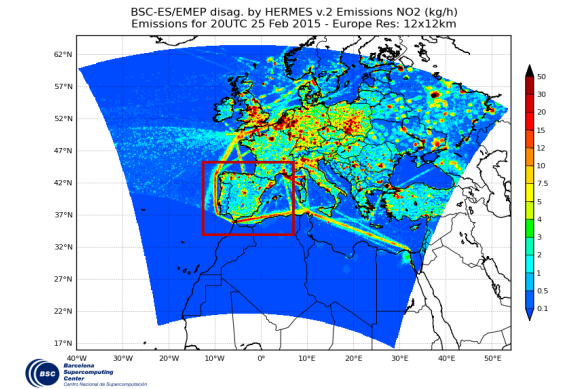
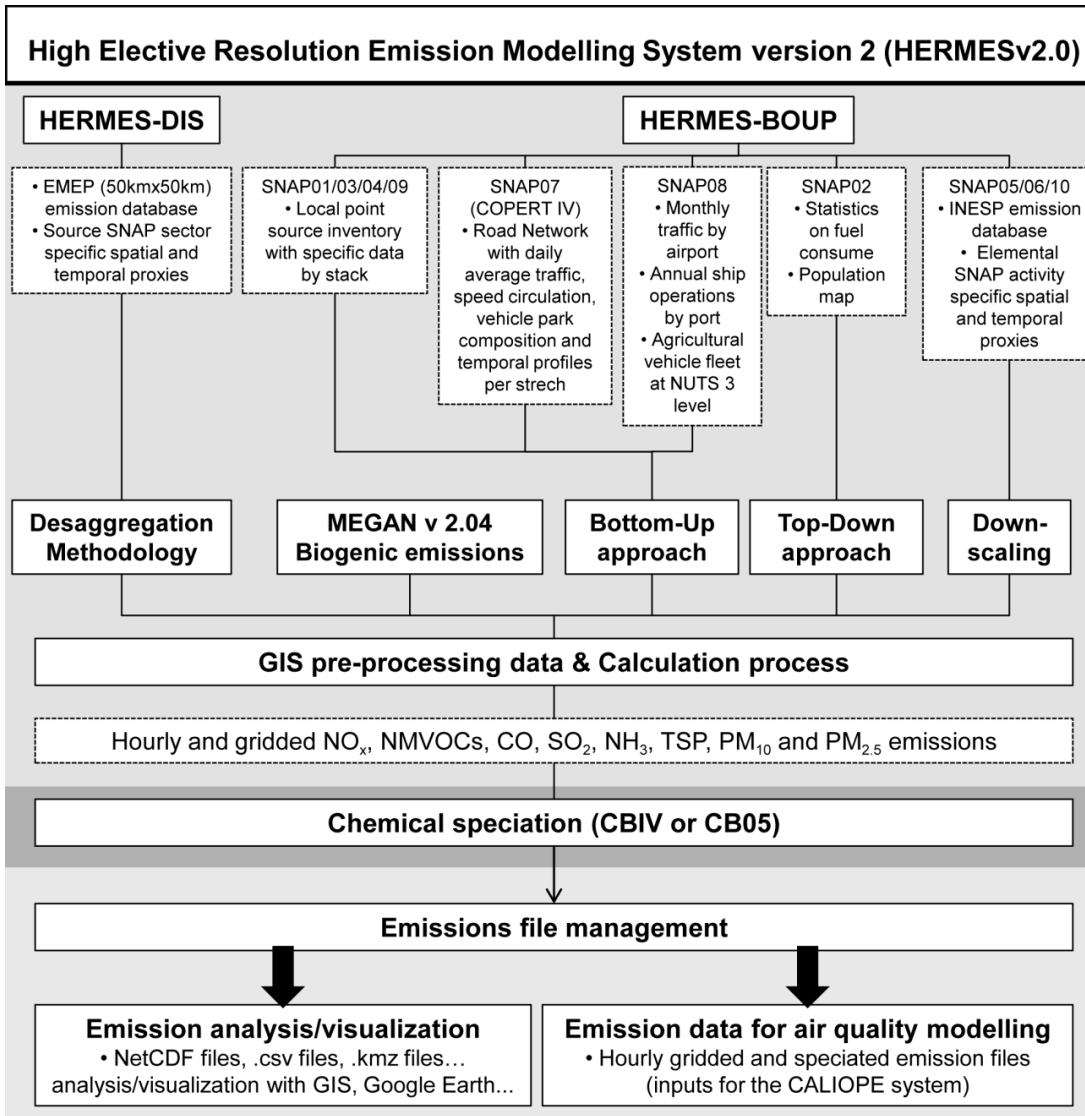


## MONARCH ongoing

- Refinement of model schemes
  - ✓ on-line natural emissions,
  - ✓ dry and wet deposition,
  - ✓ aerosol size distributions,
  - ✓ optical properties,
  - ✓ convective transport,
  - ✓ stratospheric boundary conditions.
- Missing species and processes
  - ✓ marine POA,
  - ✓ anthropogenic OA
  - ✓ dust mineral types
  - ✓ heterogeneous chemistry
  - ✓ new SOA pathways and mechanisms
- One-way nesting capabilities of the model (global-regional, regional-regional)
- 2017 -> full aerosol global forecasts
- 2018 -> transition of regional CALIOPE forecasts to MONARCH

# HERMESv2.0:

## An emission model for Europe and Spain





# HERMESv3.0: A multiscale emission model for supporting air quality modelling research



Barcelona  
Supercomputing  
Center  
Centro Nacional de Supercomputación



A stand-alone model for simulating emissions on a user-defined grid for global, regional and street-scale air quality models. Users can select, combine and scale (horizontal, vertical, temporal, speciation) multiple global and regional emission inventories through a flexible configuration file to obtain hourly gridded emissions.

## Emission data library

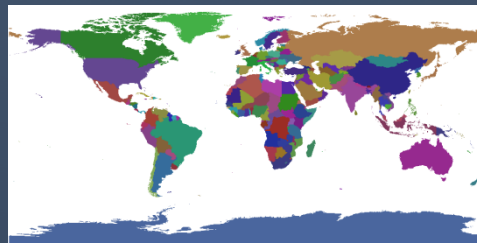
- \* Multiple global and regional emission inventories (no pre-processing needed)
- \* Online emissions:
  - Biogenic (MEGAN)
  - Lightning
  - Ocean
- \* Spanish bottom-up emission inventory (street level emissions)



(...)

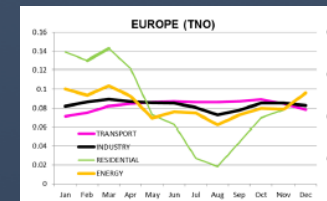
## Conservative regridding

- \* User-defined grid:
  - Regular lat-lon
  - Rotated lat-lon
  - Lambert Conformal Conic
- \* Mask and scale factors for combining and updating emission inventories

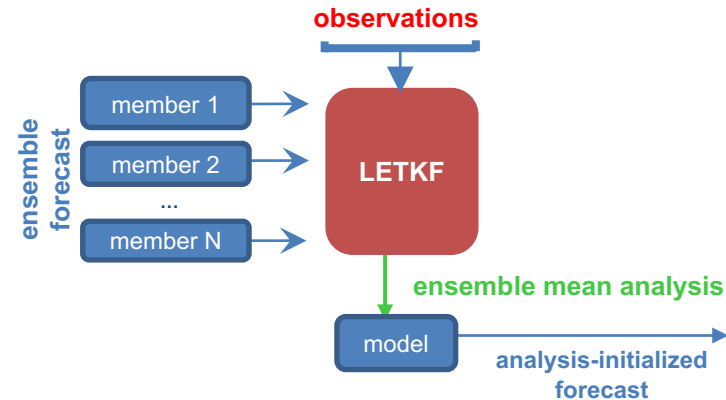


## Vertical, temporal and speciation treatment

- \* Vertical profiles:
  - Point sources
  - Biomass burning
  - Air traffic
- \* Temporal profiles: Monthly, weekly and daily factors per sector
- \* VOC and PM2.5 speciation:
  - CB05, SAPRC99
  - AERO5, AERO6



**MONARCH** coupled with a Local Ensemble Transform Kalman Filter (**LETKF**) for the assimilation of aerosol optical depth observations

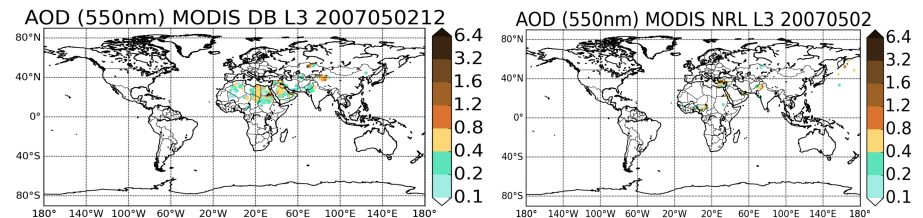


## Mineral dust application

The ensemble forecast is based on uncertainties in the dust emission scheme

- vertical flux,
- size distribution at emission
- threshold on friction velocity

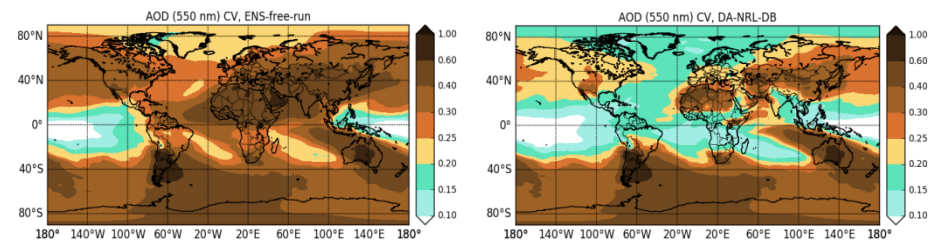
## Assimilated satellite observations, filtered for dust



*MODIS Deep Blue*

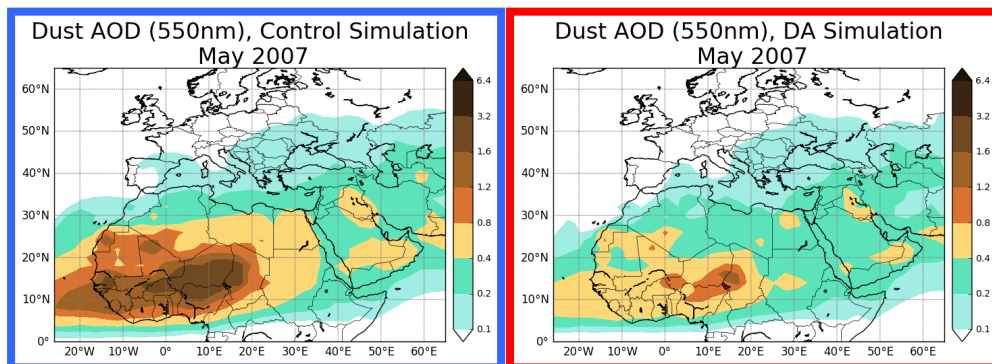
*MODIS Dark Target*

## Ensemble spread reduction where obs are present

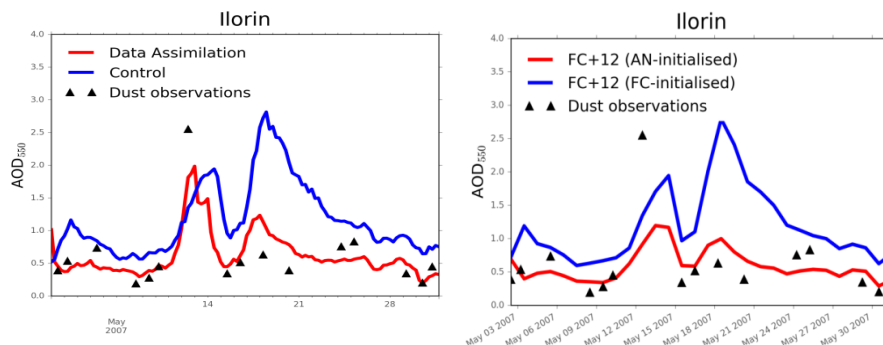


*Ensemble free run*

*DA run*



## AERONET Validation



Better description of current and forecast conditions for dust with data assimilation

## Assimilation Future

- Development of improved ensemble members (perturbed sources, model schemes and atmospheric initial conditions)
- Testing assimilation of vertical profiles (LIDAR)
- Combining multiple sources of data
- Aerosol reanalysis with data assimilation
- Multiple aerosol species (not only dust but also sea-salt, sulphate and organics)

# Mineral dust: AXA Chair on Sand and Dust Storms

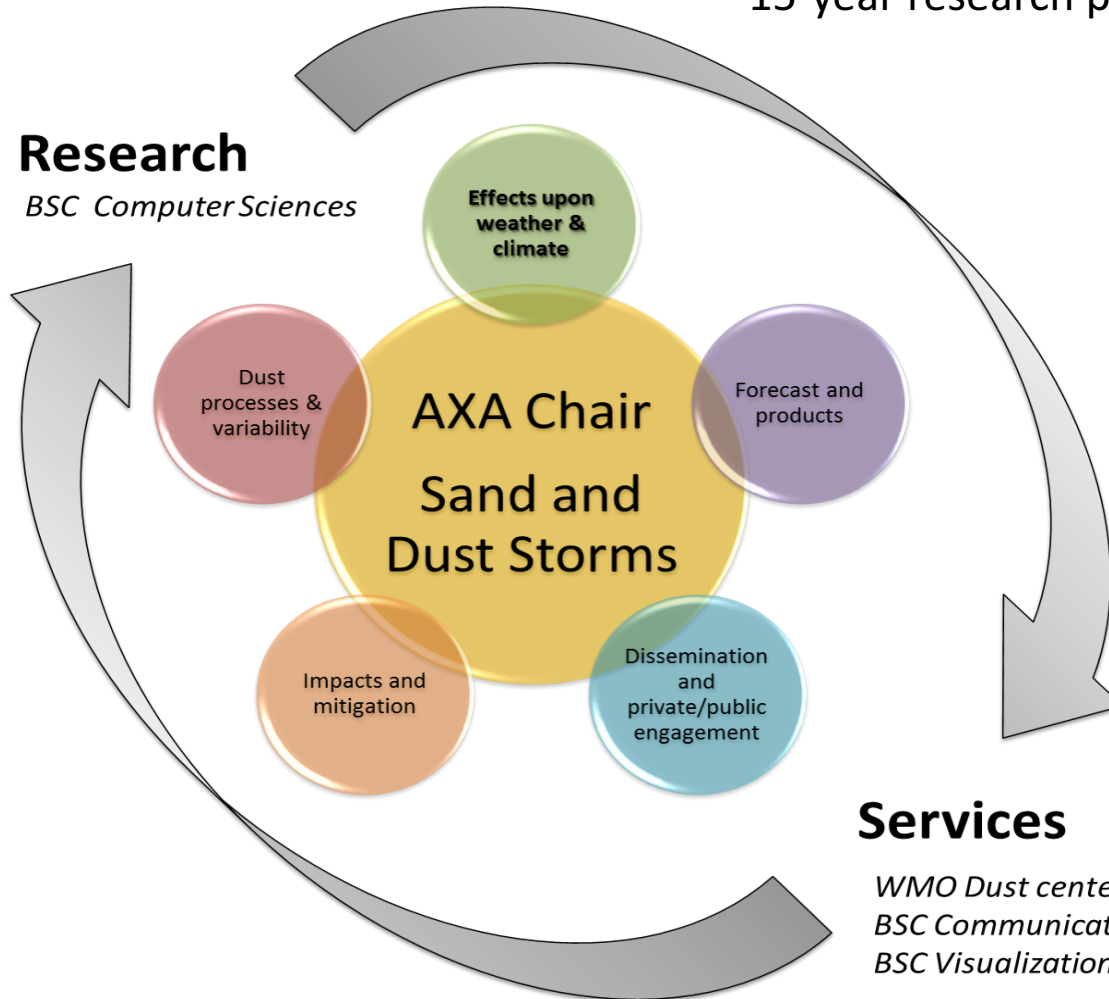


**Barcelona  
Supercomputing  
Center**  
*Centro Nacional de Supercomputación*



Started October 2016

15-year research program funded by AXA





# Mineral dust: AXA Chair on Sand and Dust Storms



**Barcelona  
Supercomputing  
Center**  
Centro Nacional de Supercomputación



## AXA CHAIR on Sand and Dust Storms

### GOALS

#### GOAL 1 DUST PROCESSES & VARIABILITY

- Present-day dust sources
- Wind gusts and dust mobilization
- Dust variability

#### GOAL 2 EFFECTS UPON WEATHER & CLIMATE

- Dust composition
- Weather and climate
- Atmospheric chemistry and iron

#### GOAL 3 FORECASTS & PRODUCTS

- Data assimilation and model evaluation
- Global and regional dust forecasting
- Ensemble dust forecasting
- Long-range dust prediction
- Dust reanalysis

#### GOAL 4 IMPACTS & MITIGATION

- Health
- Agriculture
- Solar energy and transportation

#### GOAL 5 DISSEMINATION & PUBLIC ENGAGEMENT

- Scientific community
- Industry
- National Weather Services & decision-makers
- General public

### FOCUS AREAS

### TWO-WAY GOALS INTERACTIONS

### HOST INSTITUTION: EARTH SCIENCES DEPARTMENT STRUCTURE



ATMOSPHERIC COMPOSITON GROUP

CLIMATE PREDICTION GROUP

COMPUTATIONAL EARTH SCIENCES GROUP

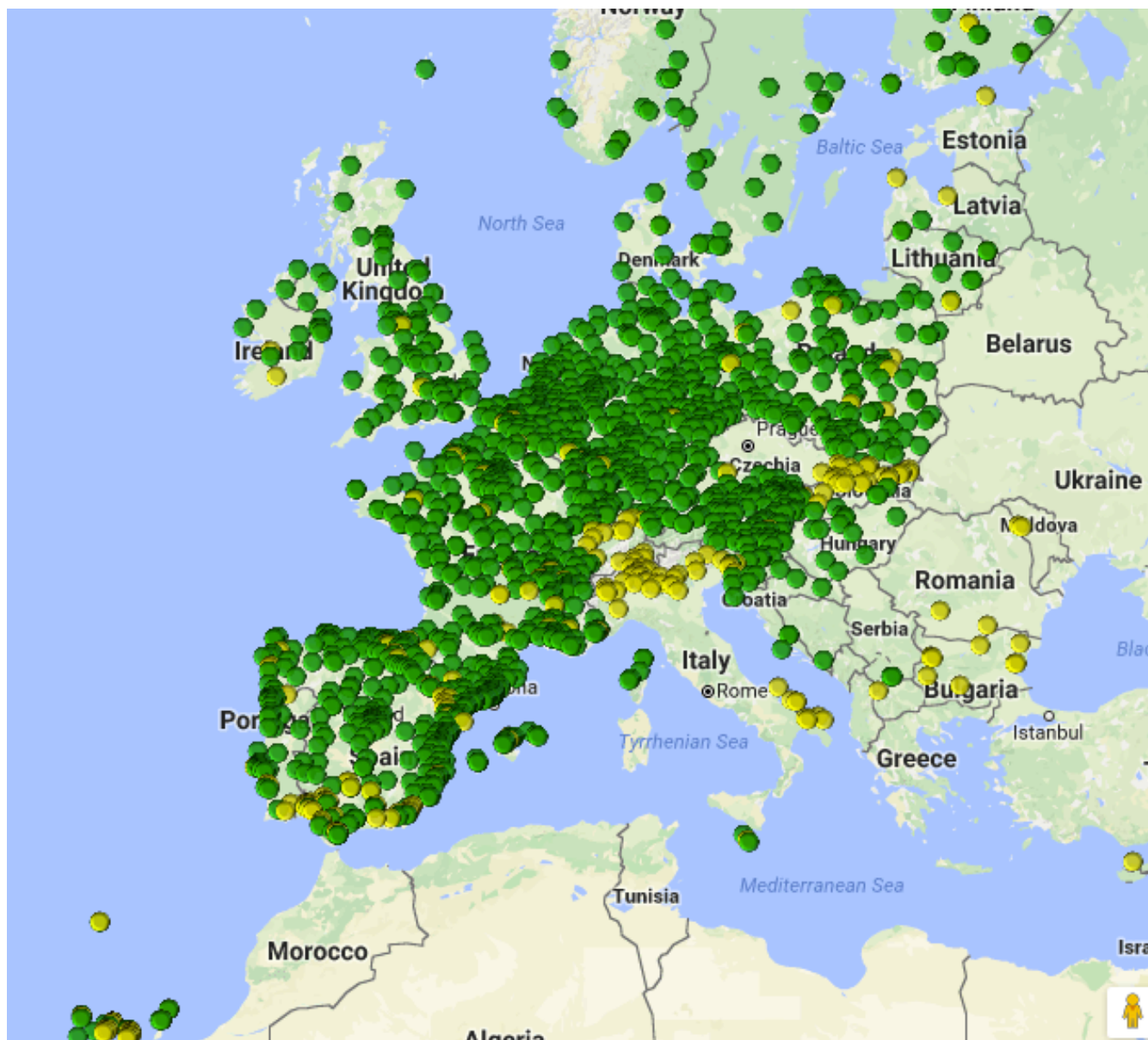
EARTH SCIENCES SERVICES GROUP

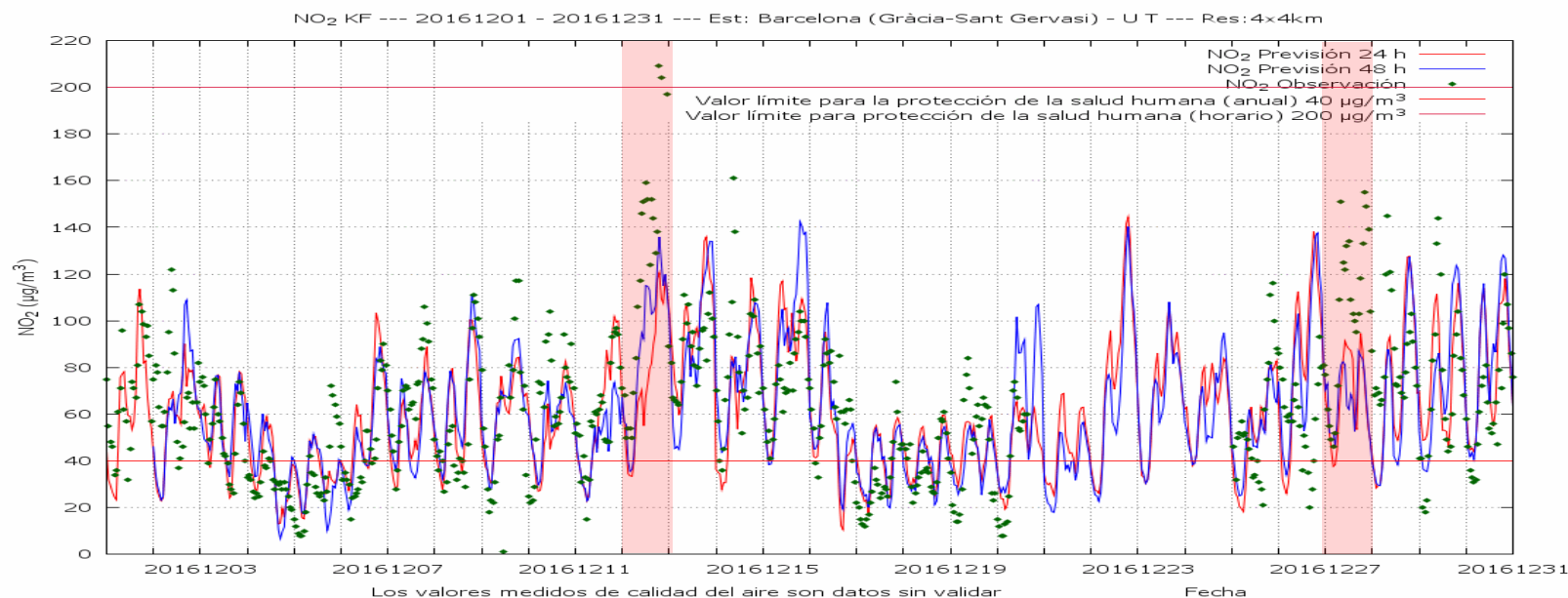
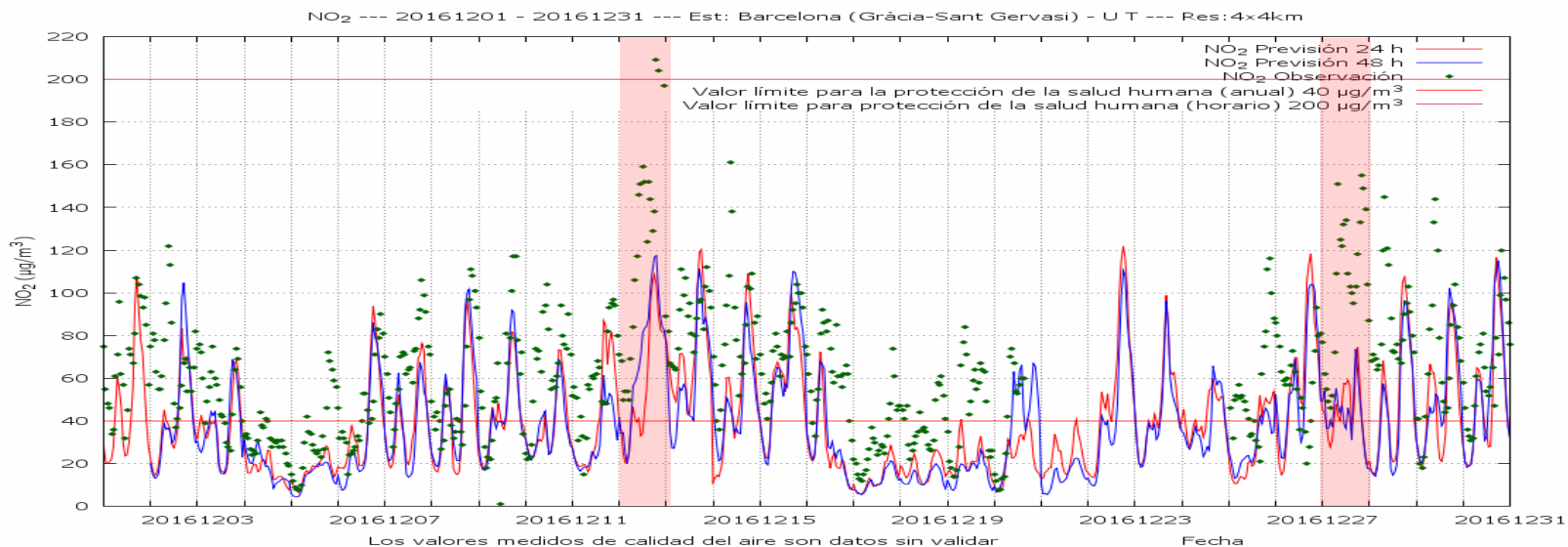
WMO SDS-WAS Regional Centers \*

BSC Communication Dpt. \*\*

\* Centers in collaboration with AEMET / \*\* Support service of the BSC-CNS to all its departments

Year	EU12	IP4	BCN1	CAT1	MAD1	AND1	CAN2
2009	100%	99%	38%	-	-	-	42%
2010	99%	99%	84%	-	-	82%	89%
2011	96%	98%	99%	-	-	98%	99%
2012	69%	49%	34%	-	-	33%	34%
2013	100%	100%	65%	54%	100%	100%	100%
2014	100%	100%	-	99%	99%	99%	100%
2015	98%	98%	-	95%	95%	95%	95%
2016	92%	92%	-	24%	24%	24%	91%





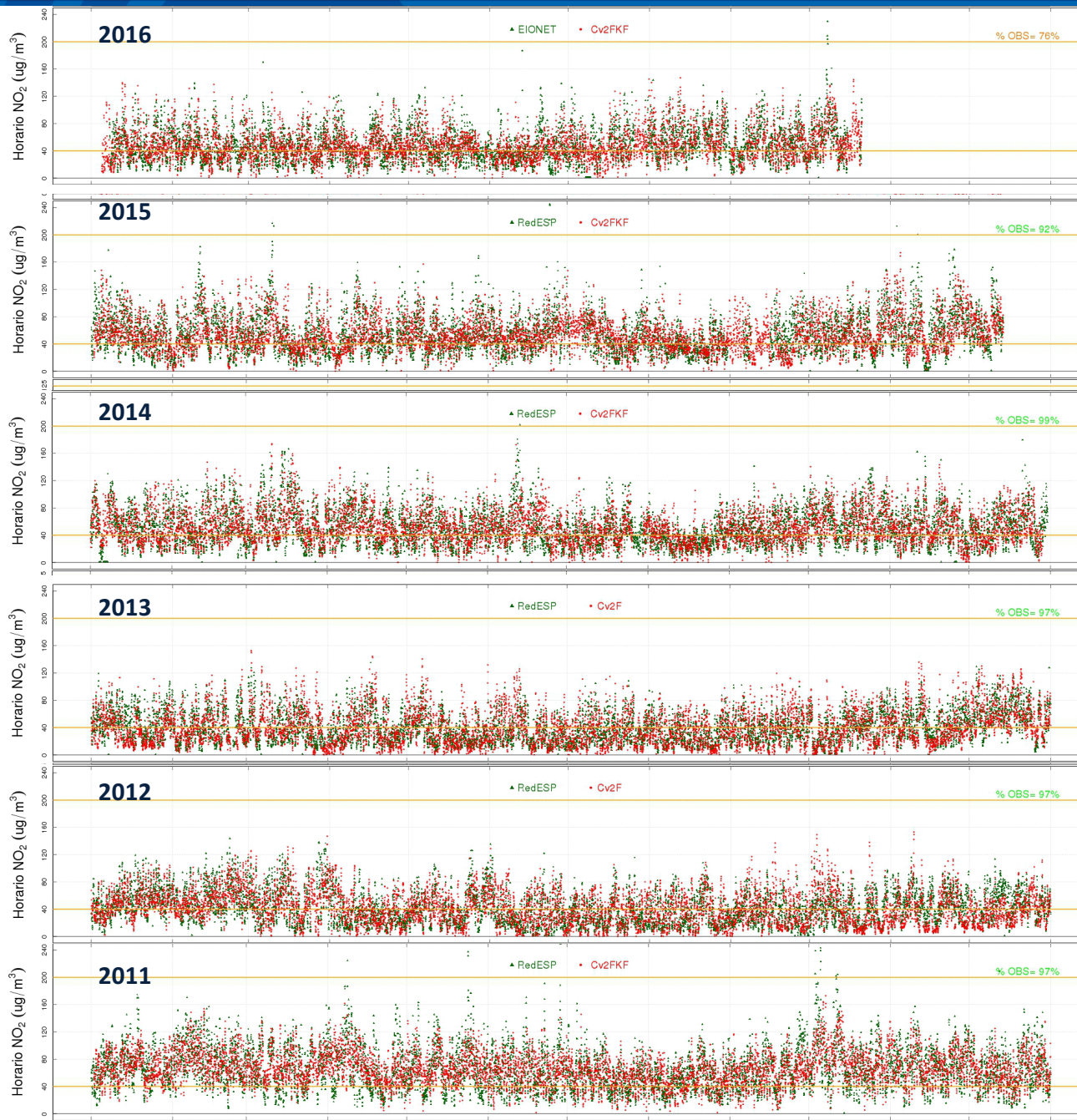
KF



# Multiyear evaluation



Barcelona  
Supercomputing



NO <sub>2</sub>	Obs media ug/m <sup>3</sup>	Mod media ug/m <sup>3</sup>	r	MB ug/m <sup>3</sup>	RMSE ug/m <sup>3</sup>	n
Anual	47.9	47.8	0.52	-0.2	23.3	8060
Ene	45.8	48.7	0.48	-0.2	24.3	242
Feb	45.8	45.9	0.59	0.0	21.1	643
Mar	43.6	44.1	0.42	0.5	22.6	720
Abr	46.6	47.6	0.45	1.0	22.8	653
May	46.6	47.7	0.38	1.0	23.2	669
Jun	40.0	39.2	0.25	-0.8	25.1	672
Jul	45.9	43.9	0.49	-2.1	25.2	564
Ago	57.9	59.3	0.47	1.5	24.1	616
Sep	48.7	47.5	0.65	-1.2	19.3	618
Oct	62.9	59.5	0.68	-3.4	25.8	373
Nov	-	-	-	-	-	-
Dic	-	-	-	-	-	-

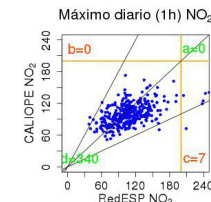
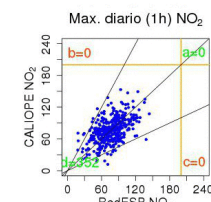
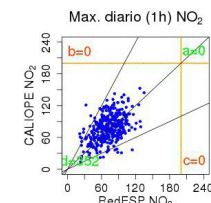
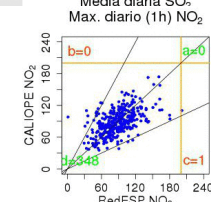
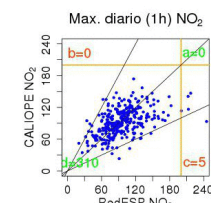
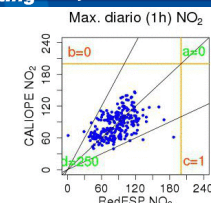
NO <sub>2</sub>	Obs media ug/m <sup>3</sup>	Mod media ug/m <sup>3</sup>	r	MB ug/m <sup>3</sup>	RMSE ug/m <sup>3</sup>	n
Anual	54.4	54.1	0.51	-0.3	26.5	7559
Ene	56.0	57.1	0.54	1.1	25.4	720
Feb	56.6	53.4	0.62	-3.2	25.8	648
Mar	51.8	53.1	0.57	1.3	26.7	740
Abr	54.6	53.6	0.40	-1.0	29.5	599
May	54.1	54.2	0.42	0.1	25.1	720
Jun	56.3	53.3	0.33	-3.0	29.1	695
Jul	48.6	52.5	0.45	3.9	24.7	605
Ago	39.8	41.4	0.43	1.6	19.3	675
Sep	52.4	41.8	0.31	-10.5	30.3	408
Oct	56.9	57.7	0.59	0.8	23.4	743
Nov	66.1	65.2	0.52	-0.9	32.3	696
Dic	63.2	67.3	0.42	4.0	25.6	309

NO <sub>2</sub>	Obs media ug/m <sup>3</sup>	Mod media ug/m <sup>3</sup>	r	MB ug/m <sup>3</sup>	RMSE ug/m <sup>3</sup>	n
Anual	51.1	51.5	0.54	0.4	24.7	8399
Ene	52.6	53.6	0.52	1.0	26.1	736
Feb	55.8	54.6	0.63	-1.2	22.6	672
Mar	57.7	58.2	0.65	0.6	27.1	741
Abr	55.2	56.1	0.44	0.9	26.4	694
May	47.9	48.9	0.45	0.9	23.4	739
Jun	52.2	54.9	0.39	2.7	30.6	692
Jul	45.0	43.2	0.44	-1.8	22.8	645
Ago	34.8	36.7	0.49	1.9	17.3	672
Sep	48.8	47.1	0.31	-1.7	23.7	720
Oct	62.3	63.2	0.44	1.0	26.7	696
Nov	48.7	49.6	0.62	0.9	23.0	709
Dic	51.4	50.6	0.48	-0.7	24.4	672

NO <sub>2</sub>	Obs media ug/m <sup>3</sup>	Mod media ug/m <sup>3</sup>	r	MB ug/m <sup>3</sup>	RMSE ug/m <sup>3</sup>	n
Anual	39.8	40.3	0.55	0.5	22.7	8464
Ene	48.4	36.5	0.59	-11.9	22.7	719
Feb	42.2	40.4	0.61	-1.8	20.6	610
Mar	40.1	46.1	0.52	6.0	25.8	655
Abr	39.4	37.5	0.48	-1.9	25.6	720
May	33.2	37.0	0.53	3.7	22.7	744
Jun	31.8	39.5	0.46	7.7	24.2	671
Jul	34.2	33.7	0.44	-0.5	22.0	742
Ago	30.3	31.5	0.53	1.1	18.4	744
Sep	36.3	33.6	0.53	-2.7	21.7	695
Oct	39.3	37.8	0.56	-1.5	21.5	744
Nov	45.0	42.5	0.58	-2.5	22.0	720
Dic	58.9	61.5	0.50	2.5	24.3	669

NO <sub>2</sub>	Obs media ug/m <sup>3</sup>	Mod media ug/m <sup>3</sup>	r	MB ug/m <sup>3</sup>	RMSE ug/m <sup>3</sup>	n
Anual	41.8	41.5	0.56	-0.2	22.9	8472
Ene	53.2	51.2	0.58	-2.0	18.7	743
Feb	57.1	58.1	0.51	0.9	23.1	674
Mar	52.8	52.3	0.57	-0.5	26.9	682
Abr	31.7	37.4	0.40	5.7	23.9	717
May	43.1	42.8	0.53	-0.3	22.6	685
Jun	31.9	37.8	0.56	5.9	23.0	720
Jul	31.0	32.7	0.56	1.7	18.5	744
Ago	33.1	34.8	0.60	1.7	20.1	744
Sep	33.9	37.5	0.45	3.6	23.1	702
Oct	37.9	40.2	0.50	2.2	26.2	719
Nov	49.9	38.3	0.54	-11.6	25.3	714
Dic	47.7	36.5	0.53	-11.2	21.7	638

NO <sub>2</sub>	Obs media ug/m <sup>3</sup>	Mod media ug/m <sup>3</sup>	r	MB ug/m <sup>3</sup>	RMSE ug/m <sup>3</sup>	n
Anual	65.9	65.8	0.53	-0.1	27.3	8413
Ene	69.6	69.5	0.43	-0.1	24.7	654
Feb	79.9	78.5	0.53	-1.4	26.3	670
Mar	68.8	69.0	0.60	0.2	24.0	682
Abr	69.5	69.6	0.42	0.3	34.4	670
May	68.3	69.0	0.37	0.8	32.2	713
Jun	61.4	61.5	0.48	0.1	28.8	718
Jul	52.7	53.7	0.44	1.1	23.5	720
Ago	49.7	50.1	0.35	0.4	23.6	741
Sep	62.9	54.1	0.50	-8.9	25.3	720
Oct	76.8	79.7	0.51	2.9	34.6	726
Nov	71.1	71.0	0.59	-0.1	23.8	665
Dic	61.7	62.1	0.60	0.5	23.3	684

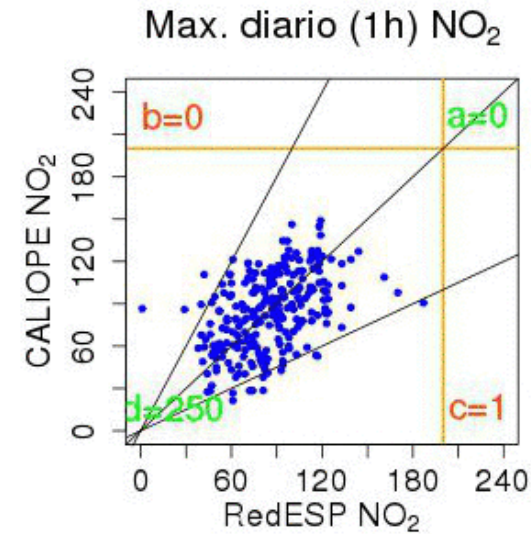




## 2016 – CALIOPE – 4 km x 4 km

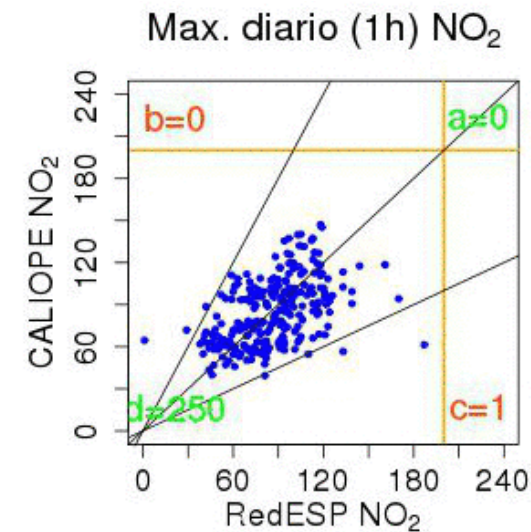
## Raw model

NO <sub>2</sub>	Obs media ug/m <sup>3</sup>	Mod media ug/m <sup>3</sup>	r	MB ug/m <sup>3</sup>	RMSE ug/m <sup>3</sup>	n
Anual	47.9	36.7	0.38	-11.3	30.0	6060
Ene	48.8	37.9	0.50	-10.9	26.6	542
Feb	45.8	34.2	0.47	-11.7	27.4	643
Mar	43.6	34.1	0.24	-9.6	29.4	720
Abr	46.6	38.6	0.21	-7.9	32.6	653
May	46.6	36.0	0.10	-10.7	32.9	669
Jun	40.0	30.9	0.15	-9.1	29.8	672
Jul	45.9	35.4	0.23	-10.6	33.5	554
Ago	57.9	48.0	0.50	-9.9	28.0	616
Sep	48.7	34.7	0.63	-14.0	24.1	618
Oct	62.9	38.8	0.64	-24.1	36.0	373
Nov	-	-	-	-	-	-
Dic	-	-	-	-	-	-



## Kalman Filter

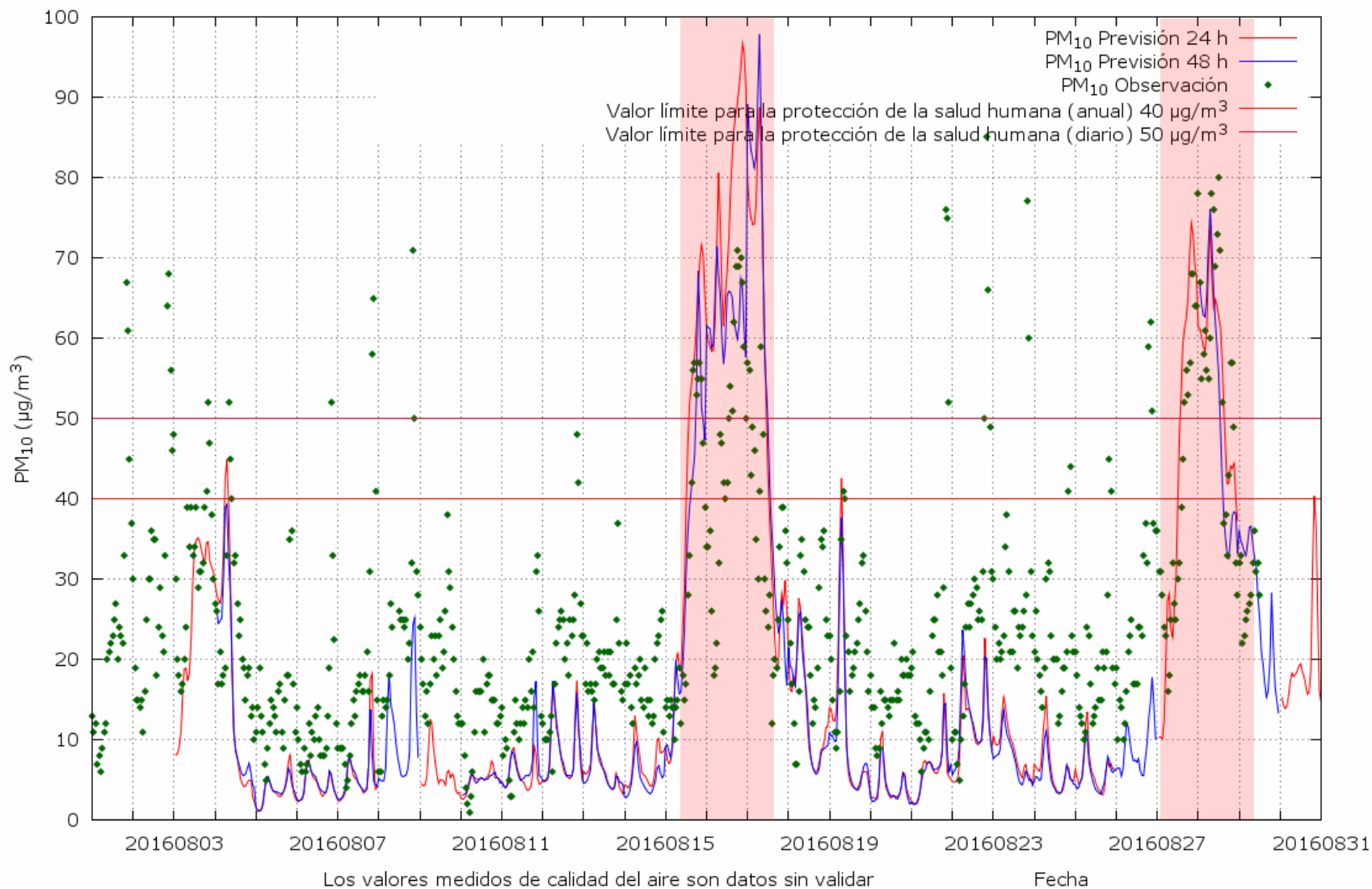
NO <sub>2</sub>	Obs media ug/m <sup>3</sup>	Mod media ug/m <sup>3</sup>	r	MB ug/m <sup>3</sup>	RMSE ug/m <sup>3</sup>	n
Anual	47.9	47.8	0.52	-0.2	23.3	6060
Ene	48.8	48.7	0.48	-0.2	24.3	542
Feb	45.8	45.9	0.59	0.0	21.1	643
Mar	43.6	44.1	0.42	0.5	22.6	720
Abr	46.6	47.6	0.45	1.0	22.8	653
May	46.6	47.7	0.38	1.0	23.2	669
Jun	40.0	39.2	0.25	-0.8	25.1	672
Jul	45.9	43.9	0.49	-2.1	25.2	554
Ago	57.9	59.3	0.47	1.5	24.1	616
Sep	48.7	47.5	0.65	-1.2	19.3	618
Oct	62.9	59.5	0.68	-3.4	25.8	373
Nov	-	-	-	-	-	-
Dic	-	-	-	-	-	-



# PM10 dust contributions



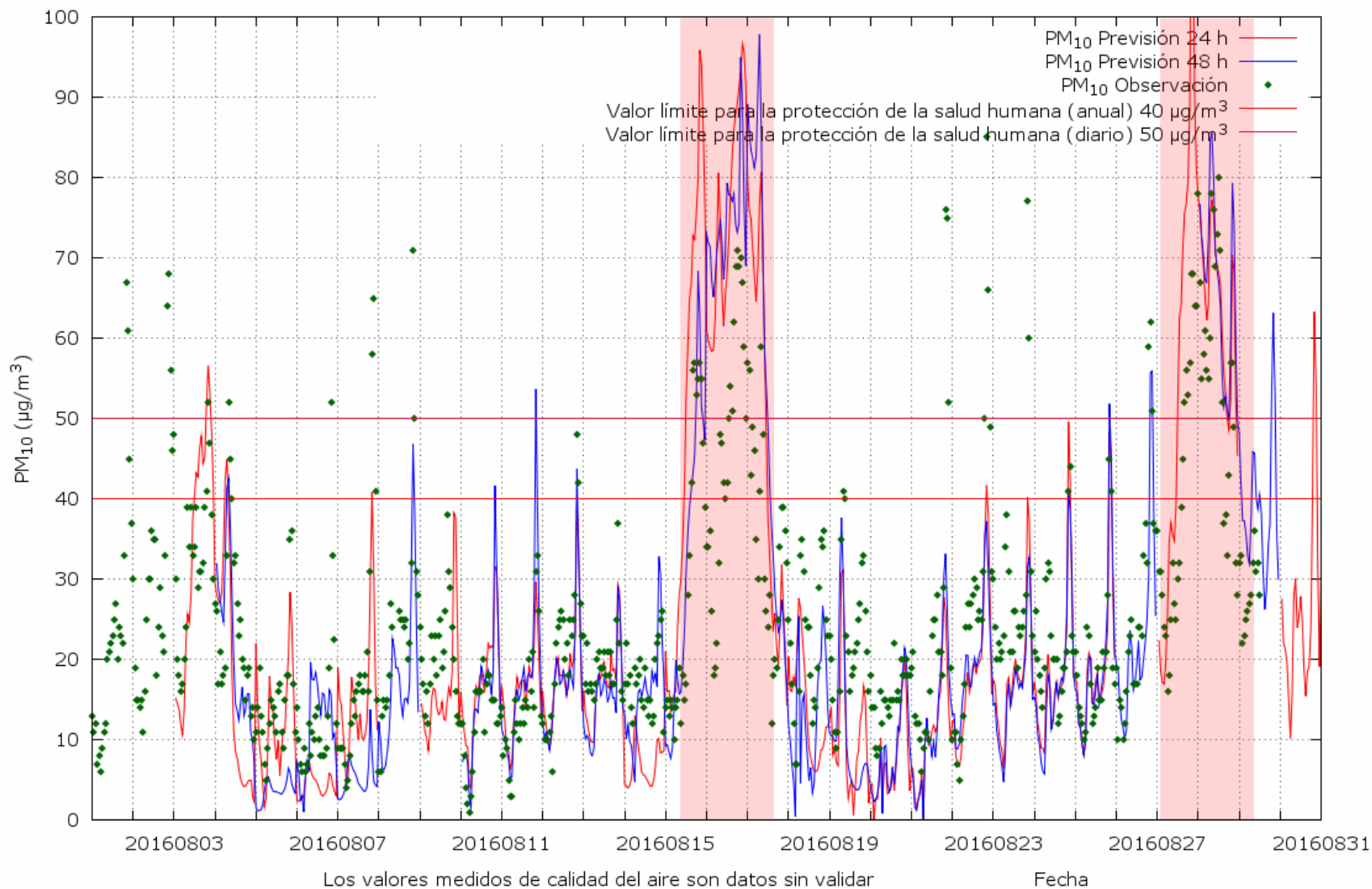
PM<sub>10</sub> --- 20160801 - 20160831 --- Est: Madrid (Escuelas Aguirre) - U T --- Res:4x4km



# PM10 dust contributions

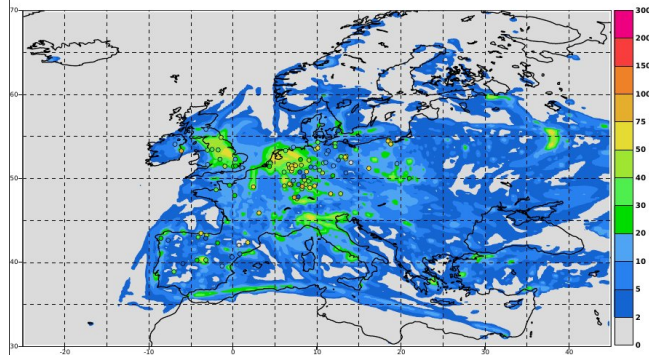


PM<sub>10</sub> KF --- 20160801 - 20160831 --- Est: Madrid (Escuelas Aguirre) - U T --- Res:4x4km

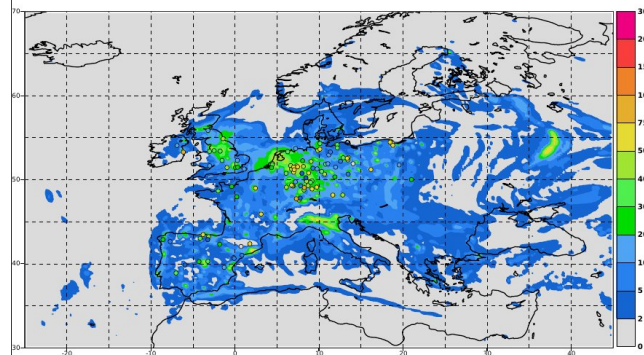




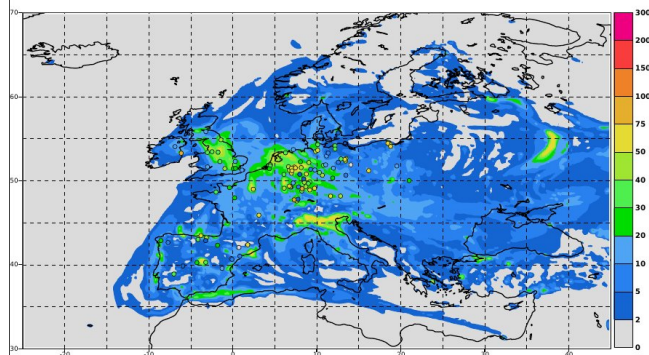
Tuesday 13 December 2016 00UTC CAMS Verification t-006 VT: Monday 12 December 2016 18UTC  
Observations + LOTOS-EUROS Analysis Surface Nitrogen Dioxide [  $\mu\text{g}/\text{m}^3$  ]



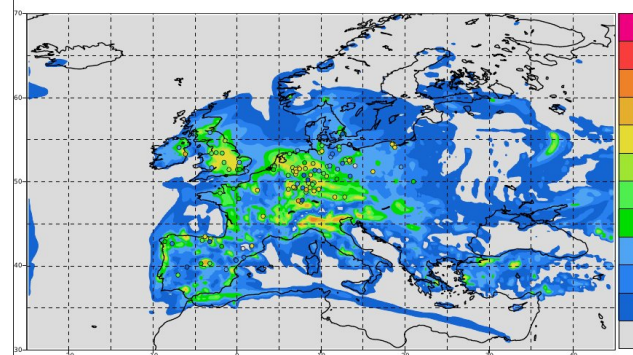
Tuesday 13 December 2016 00UTC CAMS Verification t-006 VT: Monday 12 December 2016 18UTC  
Observations + EURAD-IM Analysis Surface Nitrogen Dioxide [  $\mu\text{g}/\text{m}^3$  ]



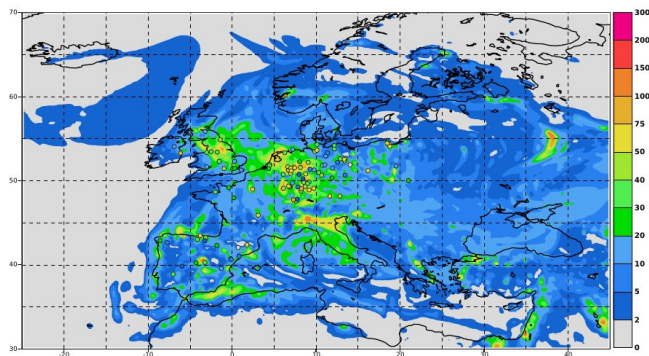
Tuesday 13 December 2016 00UTC CAMS Verification t-006 VT: Monday 12 December 2016 18UTC  
Observations + EMEP Analysis Surface Nitrogen Dioxide [  $\mu\text{g}/\text{m}^3$  ]



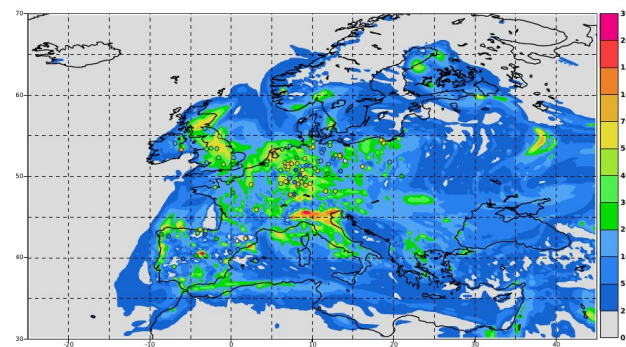
Tuesday 13 December 2016 00UTC CAMS Verification t-006 VT: Monday 12 December 2016 18UTC  
Observations + MATCH Analysis Surface Nitrogen Dioxide [  $\mu\text{g}/\text{m}^3$  ]



Tuesday 13 December 2016 00UTC CAMS Verification t-006 VT: Monday 12 December 2016 18UTC  
Observations + MOCAGE Analysis Surface Nitrogen Dioxide [  $\mu\text{g}/\text{m}^3$  ]



Tuesday 13 December 2016 00UTC CAMS Verification t-006 VT: Monday 12 December 2016 18UTC  
Observations + SILAM Analysis Surface Nitrogen Dioxide [  $\mu\text{g}/\text{m}^3$  ]

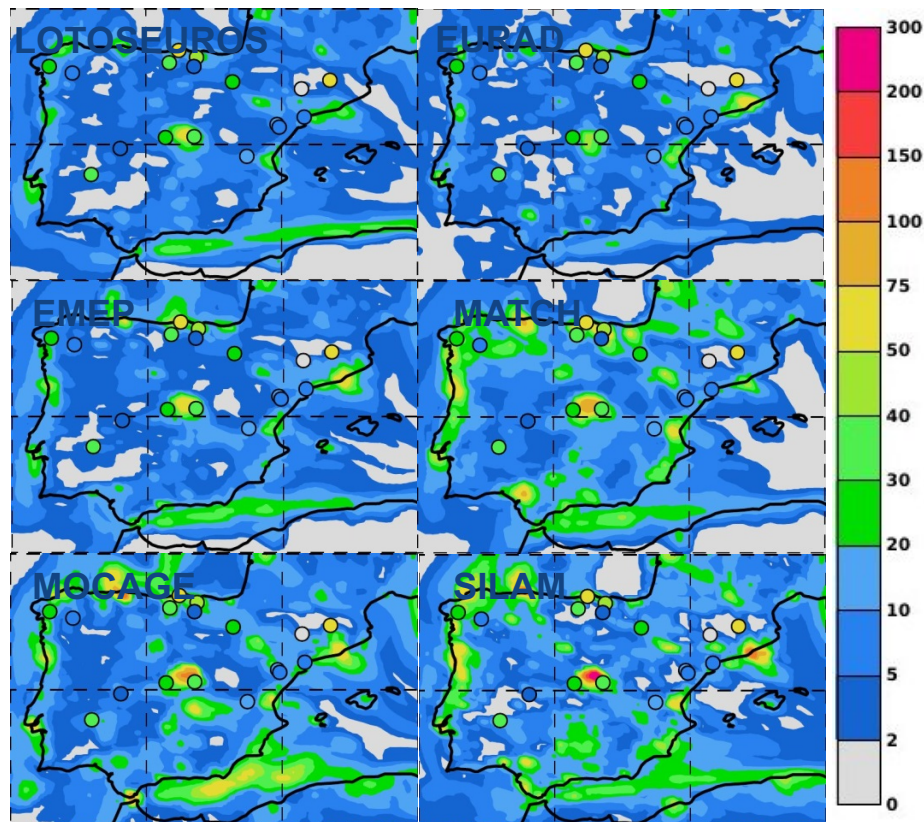


12 Dic 2015  
18 UTC  
NO<sub>2</sub>  
COPERNICUS

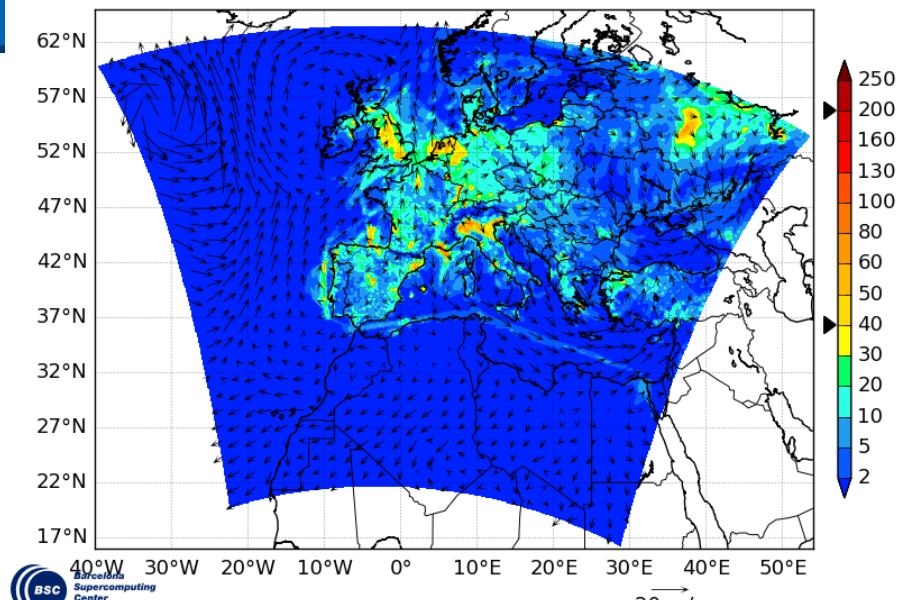


# RESOLUTION

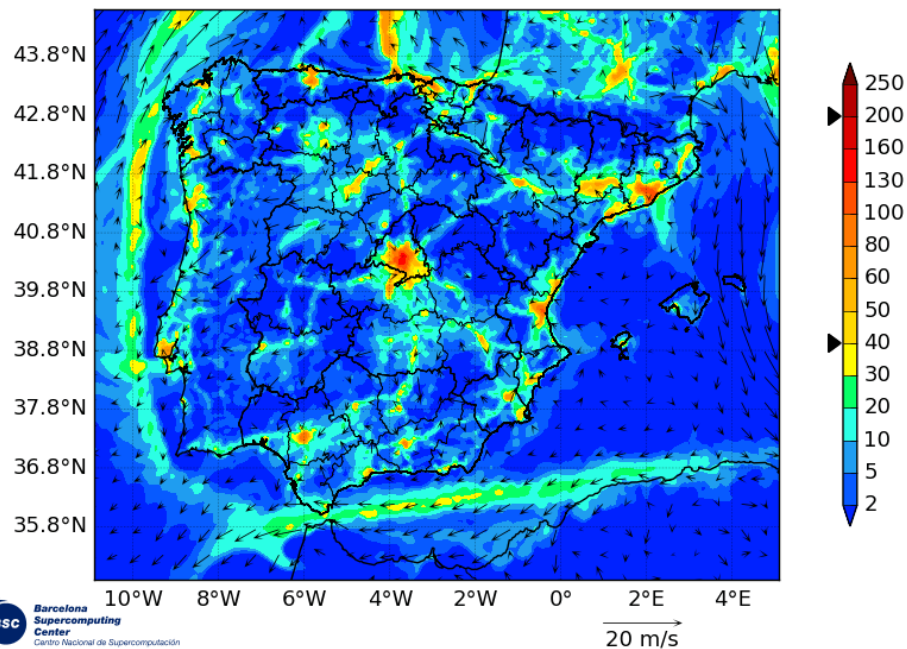
CAMS Monday 12 Dec 2016 18UTC – NO2



BSC-ES/AQF WRFv3.5.1+CMAQv5.0.2+HERMESv2 Nitrogen Dioxide ( $\mu\text{g}/\text{m}^3$ )  
42h forecast for 18UTC 12 Dec 2016 - Europe Res: 12x12km



BSC-ES/AQF WRFv3.5.1+CMAQv5.0.2+HERMESv2 Nitrogen Dioxide ( $\mu\text{g}/\text{m}^3$ )  
42h forecast for 18UTC 12 Dec 2016 - Iberian Peninsula Res: 4x4km

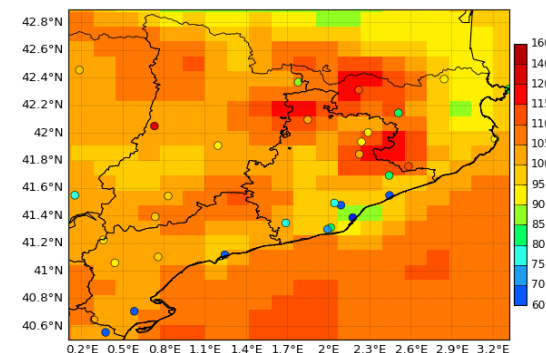
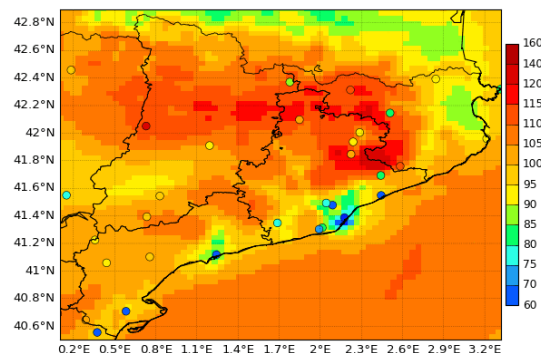
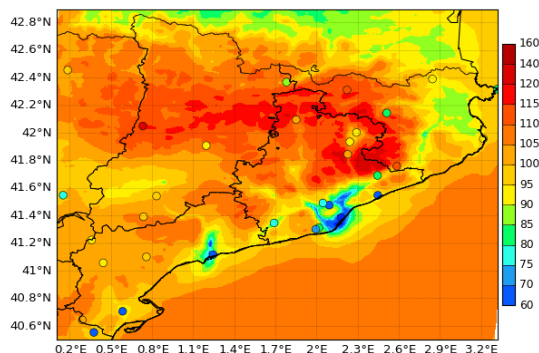
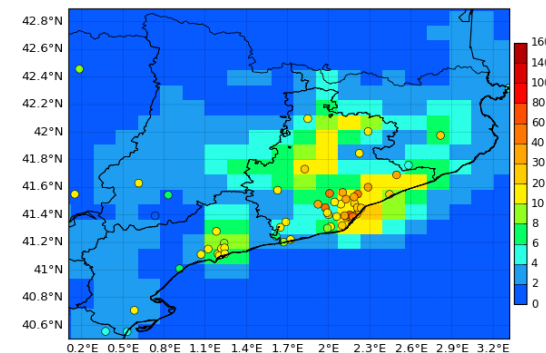
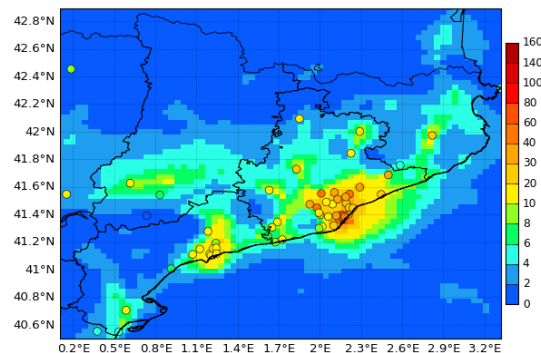
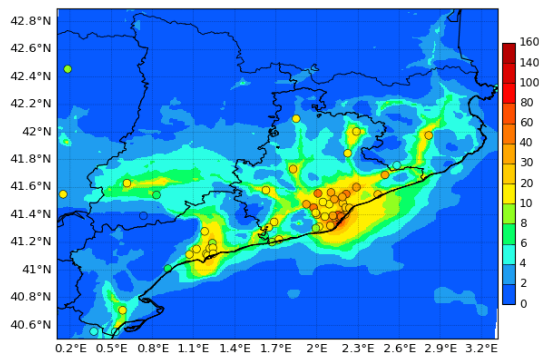


## Daily mean for the ozone episode 06-07-2015 to 18-07-2015

1 km

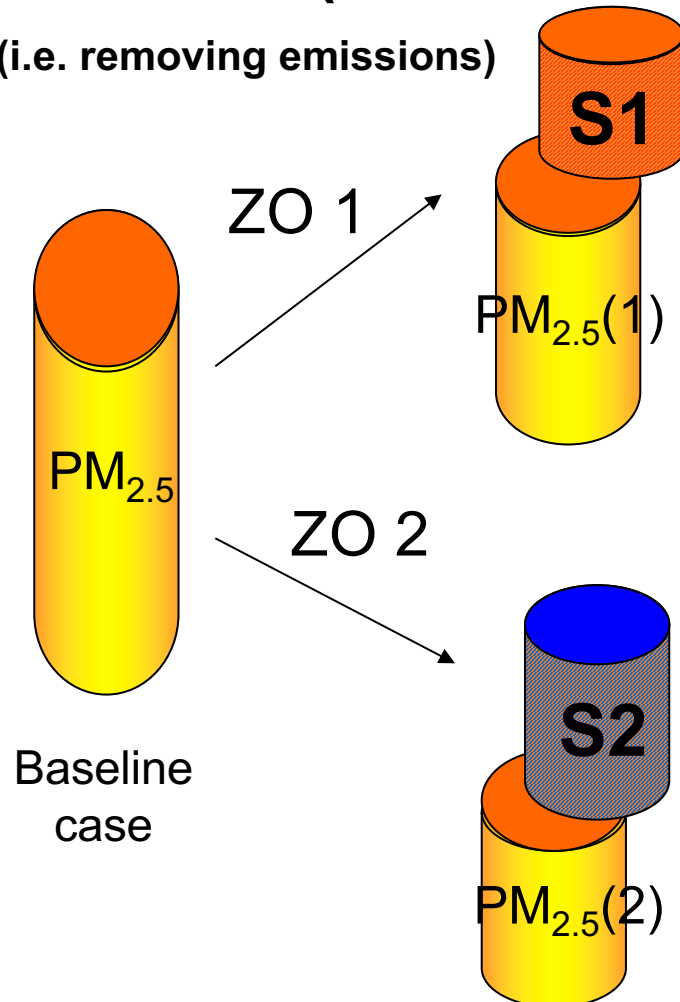
4 km

12 km

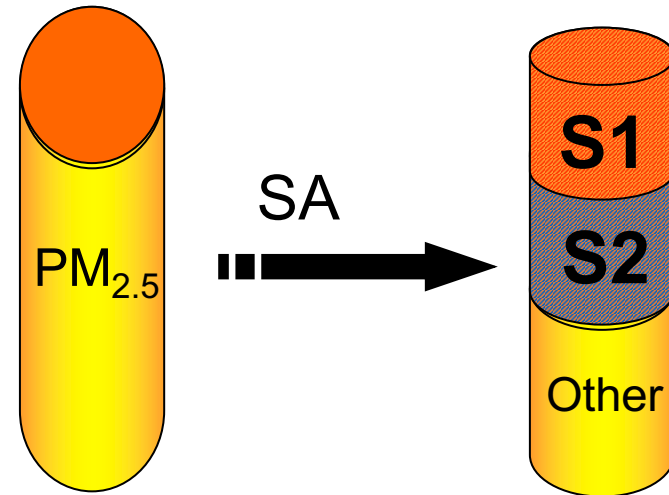
 $O_3$  $NO_2$ 

## Zero-out (brute force)

(i.e. removing emissions)



## Source apportionment (SA)

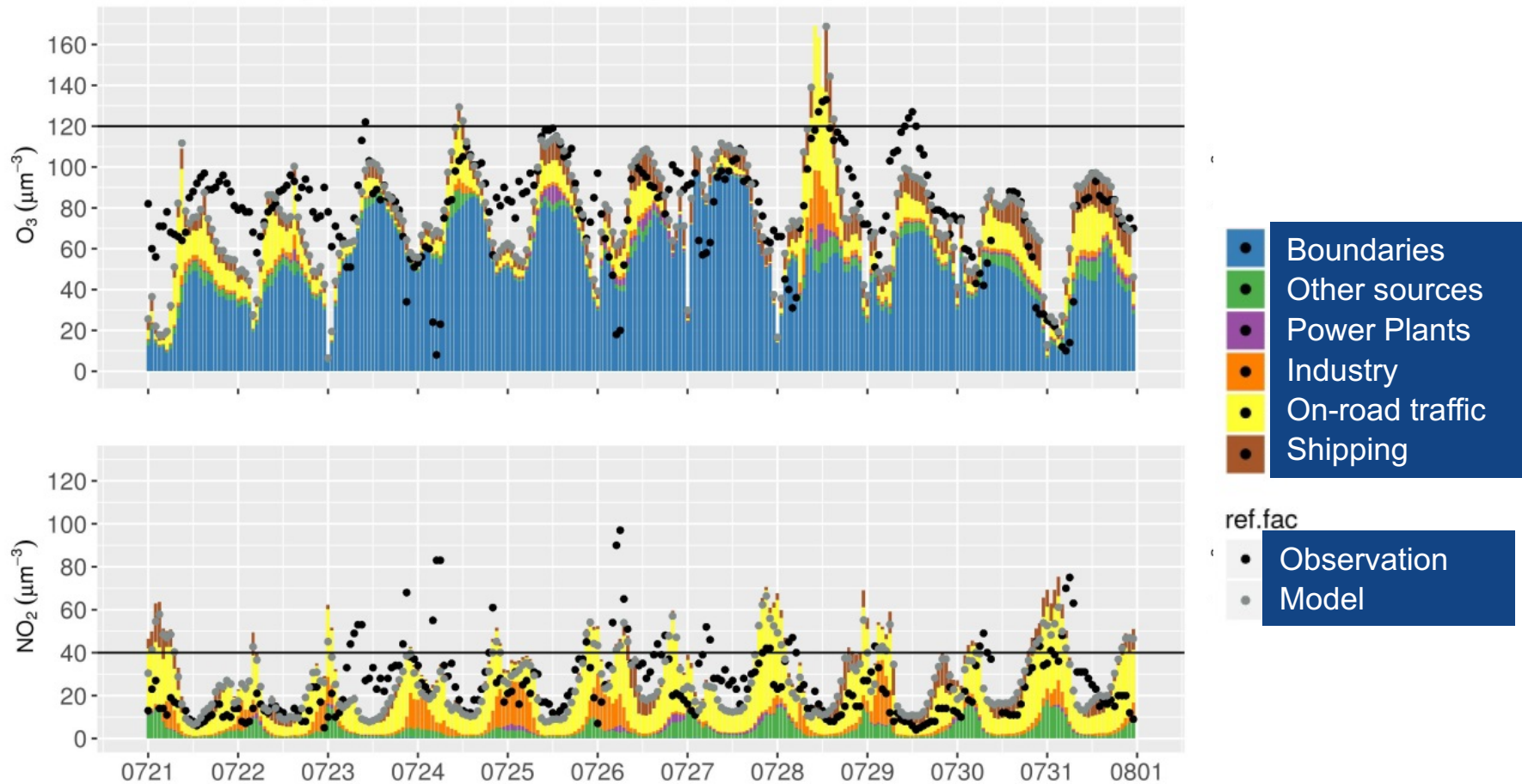


### SA advantages

- Time saving (one simulation)
- Mass consistency
- Real atmospheric conditions
- Fully traceable



(a) ES1992A-BARCELONA (PALAU REAL) - BAC-URB



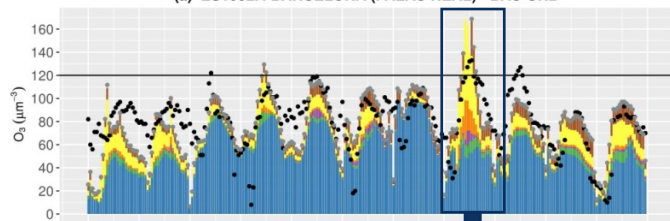
# SA for ozone



**Barcelona Supercomputing Center**  
Centro Nacional de Supercomputación



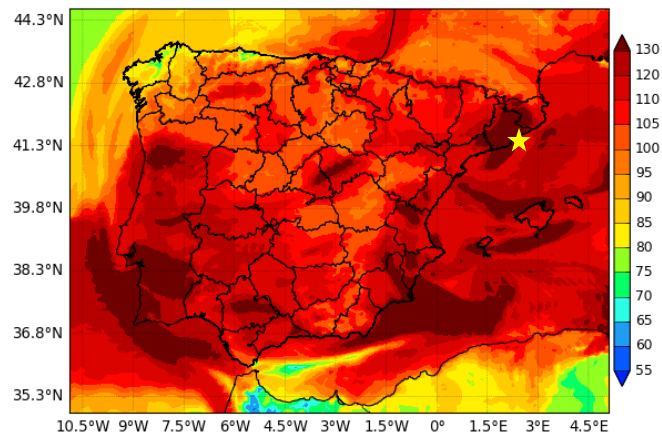
(a) ES1992A-BARCELONA (PALAU REAL) - BAC-URB



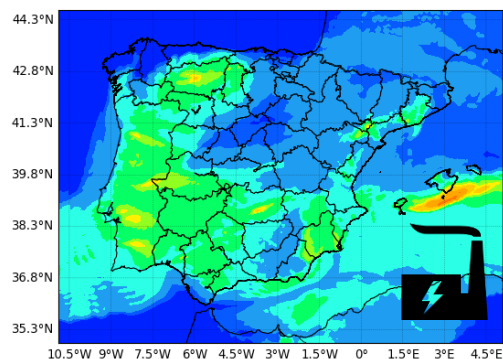
28 July 2012

**NET O<sub>3</sub>**

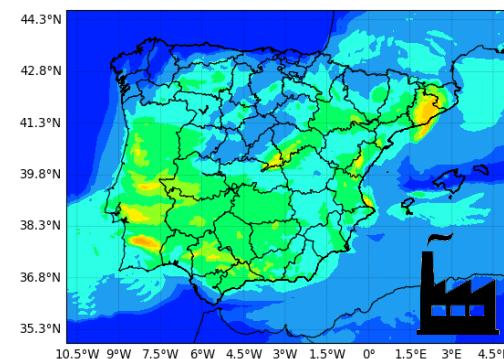
BSC-ES/AQF ARWv3+CMAQ-ISAM+HERMESv2 O<sub>3</sub> (µg/m³)  
p90 forecast for 28 Jul 2012 - Res:4x4km



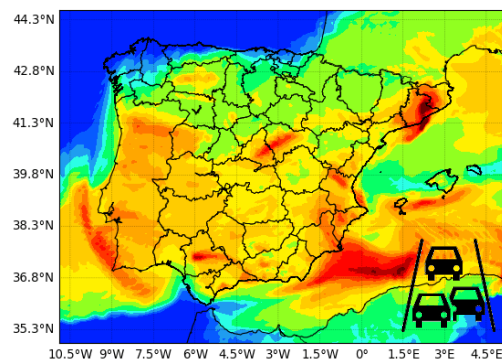
BSC-ES/AQF ARWv3+CMAQ-ISAM+HERMESv2 O<sub>3</sub> SNAP1 (µg/m³)  
p90 forecast for 28 Jul 2012 - Res:4x4km



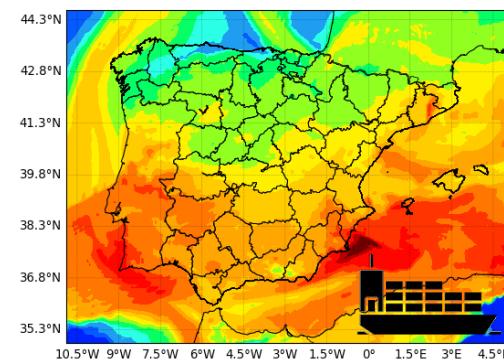
BSC-ES/AQF ARWv3+CMAQ-ISAM+HERMESv2 O<sub>3</sub> SNAP34 (µg/m³)  
p90 forecast for 28 Jul 2012 - Res:4x4km



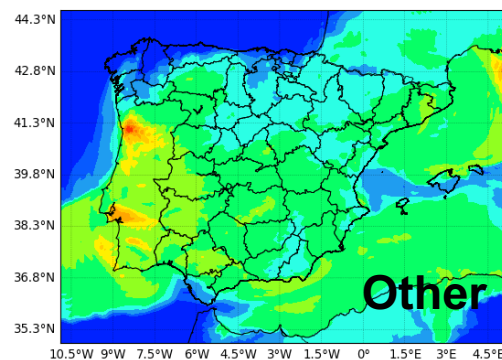
BSC-ES/AQF ARWv3+CMAQ-ISAM+HERMESv2 O<sub>3</sub> SNAP7 (µg/m³)  
p90 forecast for 28 Jul 2012 - Res:4x4km



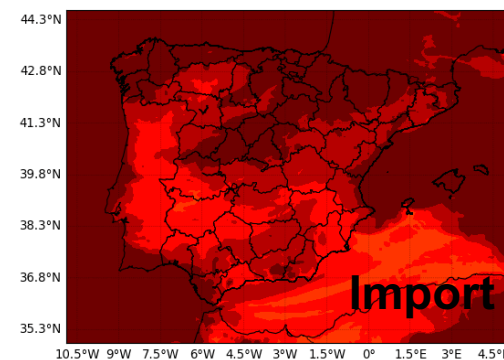
BSC-ES/AQF ARWv3+CMAQ-ISAM+HERMESv2 O<sub>3</sub> SNAP8 (µg/m³)  
p90 forecast for 28 Jul 2012 - Res:4x4km



BSC-ES/AQF ARWv3+CMAQ-ISAM+HERMESv2 O<sub>3</sub> OTHER (µg/m³)  
p90 forecast for 28 Jul 2012 - Res:4x4km



BSC-ES/AQF ARWv3+CMAQ-ISAM+HERMESv2 O<sub>3</sub> BCON (µg/m³)  
p90 forecast for 28 Jul 2012 - Res:4x4km



## Earth System Services

The Earth System Services group facilitates technology transfer of state-of-the-art research from local, national to international levels





## RESEARCH

Air quality

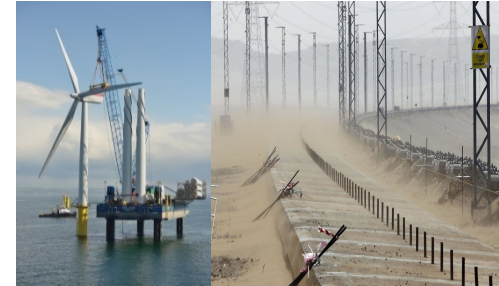
Sand  
and dust storms

Climate predictions

## USER SECTORS



Urban development



Infrastructures



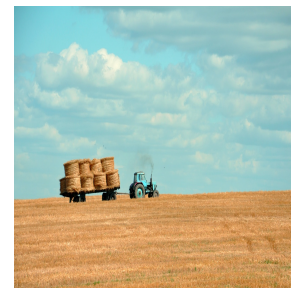
Solar energy



Transport



Wind energy



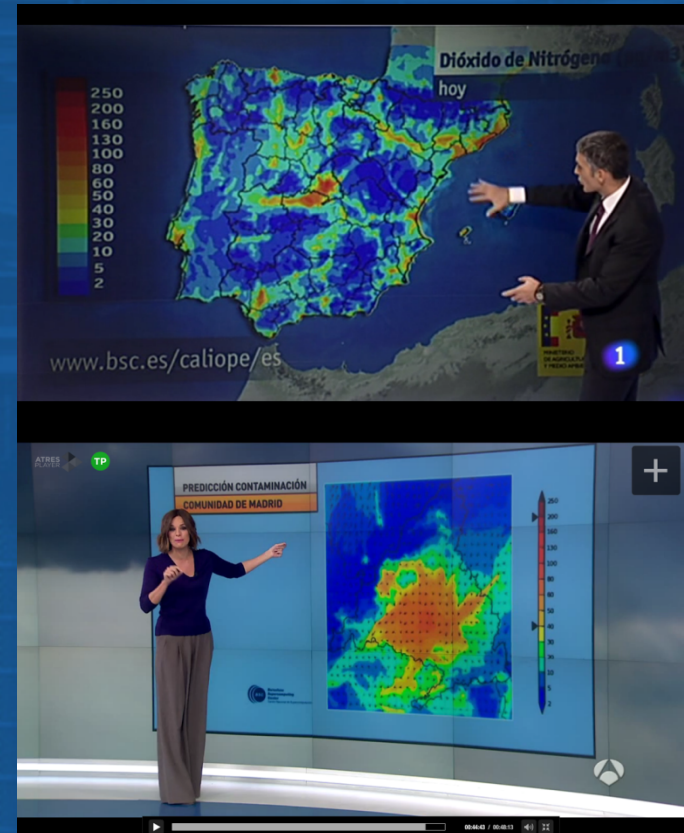
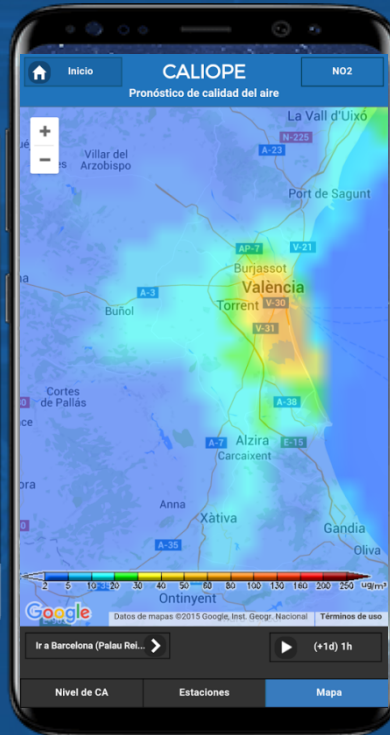
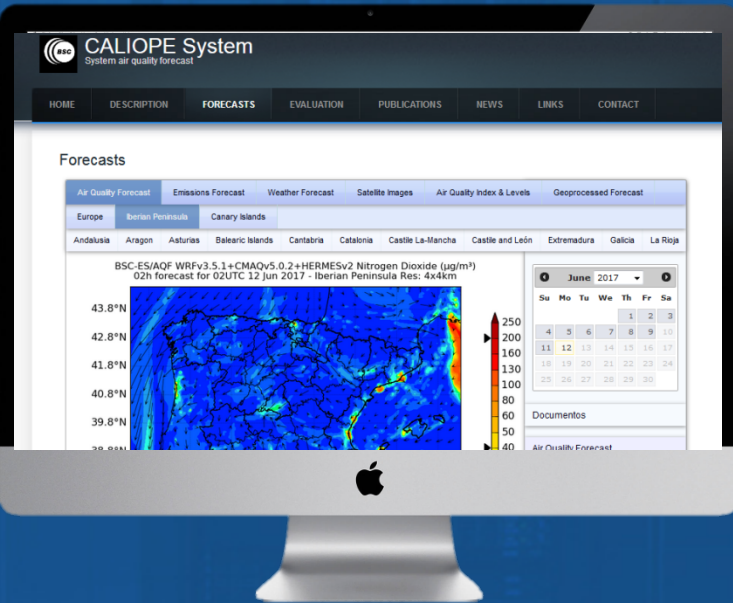
Agriculture



Insurance



# Operational forecast: CALIOPE and SDS-WAS



# CALIOPE Air quality forecast system



**Barcelona Supercomputing Center**  
Centro Nacional de Supercomputación



## CALIOPE

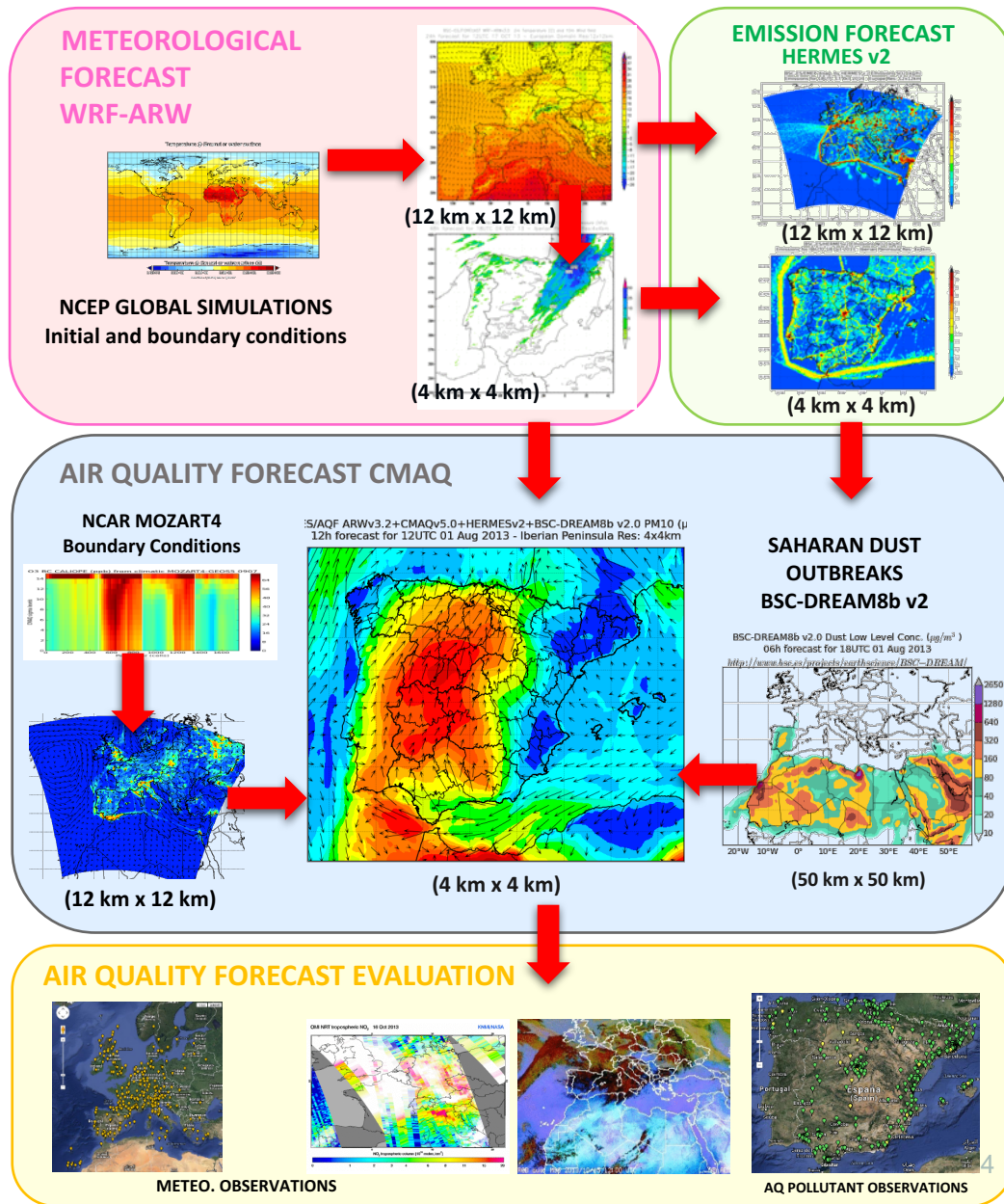
([www.bsc.es/caliope](http://www.bsc.es/caliope))

- Quantify relation between emissions, meteorology and air concentration
- Forecast air pollution episodes
- Provide and develop short and long term mitigation plans

## Domains:

**Europe** (12 km, 480 x 400 cells)

**Spain** (4 km, 399 x 399 cells)



CONSEJERÍA DE MEDIO AMBIENTE  
Y ORDENACIÓN DEL TERRITORIO



GOBIERNO DE ESPAÑA  
MINISTERIO DE AGRICULTURA, ALIMENTACIÓN  
Y MEDIO AMBIENTE



Gobierno de Canarias  
un solo pueblo

Consejería de Educación,  
Universidades y Sostenibilidad



Generalitat de Catalunya  
Departament de Territori  
i Sostenibilitat

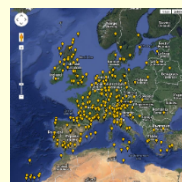


**EPRI**

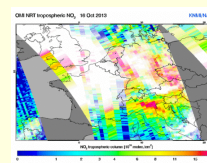


**IBERDROLA**

fundación  
**gasNatural**  
fenosa



METEO. OBSERVATIONS



AQ POLLUTANT OBSERVATIONS



# Air Quality Forecast System for Mexico DF



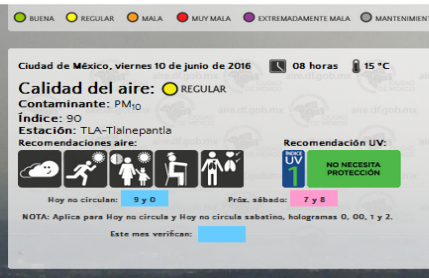
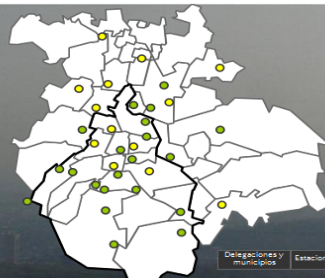
**Barcelona  
Supercomputing  
Center**  
Centro Nacional de Supercomputación



## Current Status



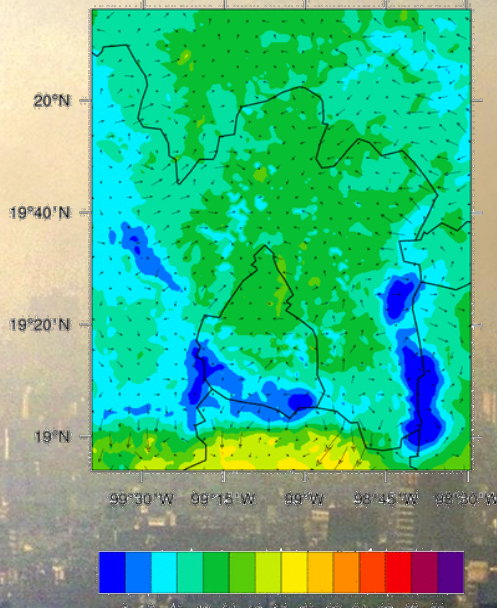
**CDMX**  
CIUDAD DE MÉXICO



Programa para mejorar la calidad del aire  
de la Zona Metropolitana  
del Valle de México  
2011-2020

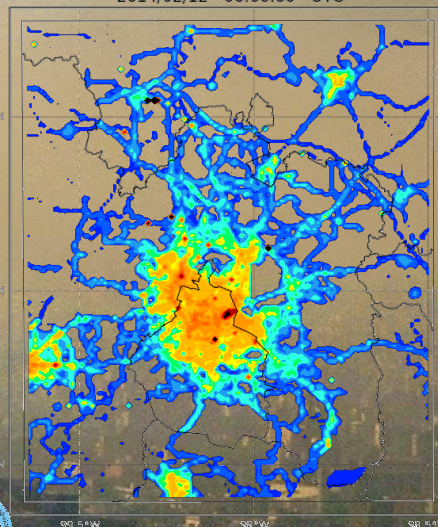


## Meteorology



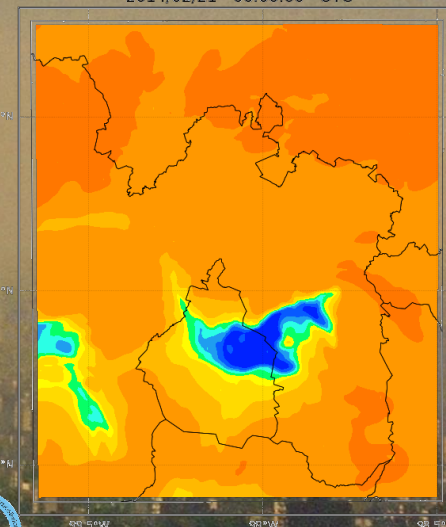
## Emissions

AQFS-MexDF NOx (kg/h) ZMVM Res:1kmx1km  
2014/02/12 - 06:00:00 - UTC



## Chemistry and Transport

AQFS-MexDF O3 (ppbV) ZMVM Res:1kmx1km  
2014/02/21 - 06:00:00 - UTC



- ✓ Complement the public information service provided by the monitoring network
- ✓ Know in advance the possibility that air pollution episodes occur
- ✓ Contribute to the development and evaluation of air quality plans (ProAire)

- ✓ Daily dust operational forecast (global and regional)

<http://www.bsc.es/earth-sciences/mineral-dust/nmmbbsc-dust-forecast>

- ✓ Contribution to the ICAP multi-model ensemble (global)

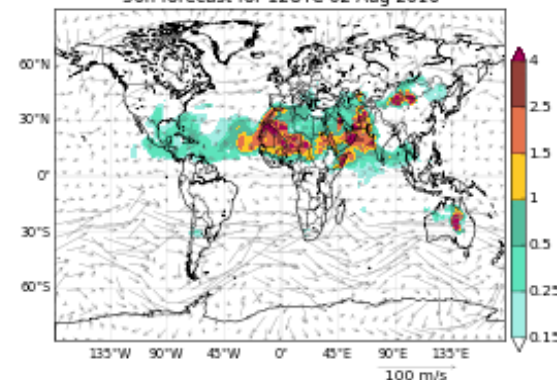
<http://icap.atmos.und.edu>

- ✓ **WMO Dust Centers**

- Sand and Dust Storm Warning Advisory and Assessment System Regional Center for North Africa, Middle East and Europe (SDS-WAS RC) <http://sds-was.aemet.es>
- Barcelona Dust Forecast Center (BSFC): First specialized WMO Center for mineral dust prediction <http://dust.aemet.es>

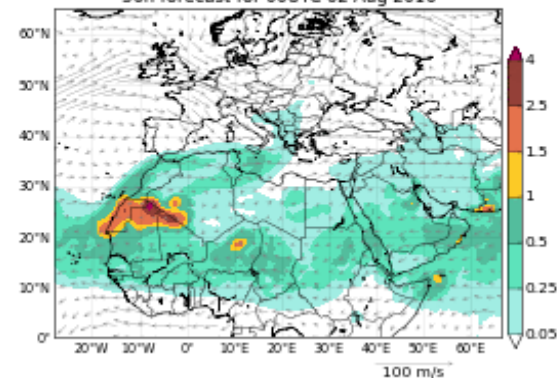
GLOBAL

NMMB/BSC-Dust Dust Load ( $\text{g}/\text{m}^2$ ) and 700 hPa Wind  
36h forecast for 12UTC 02 Aug 2016

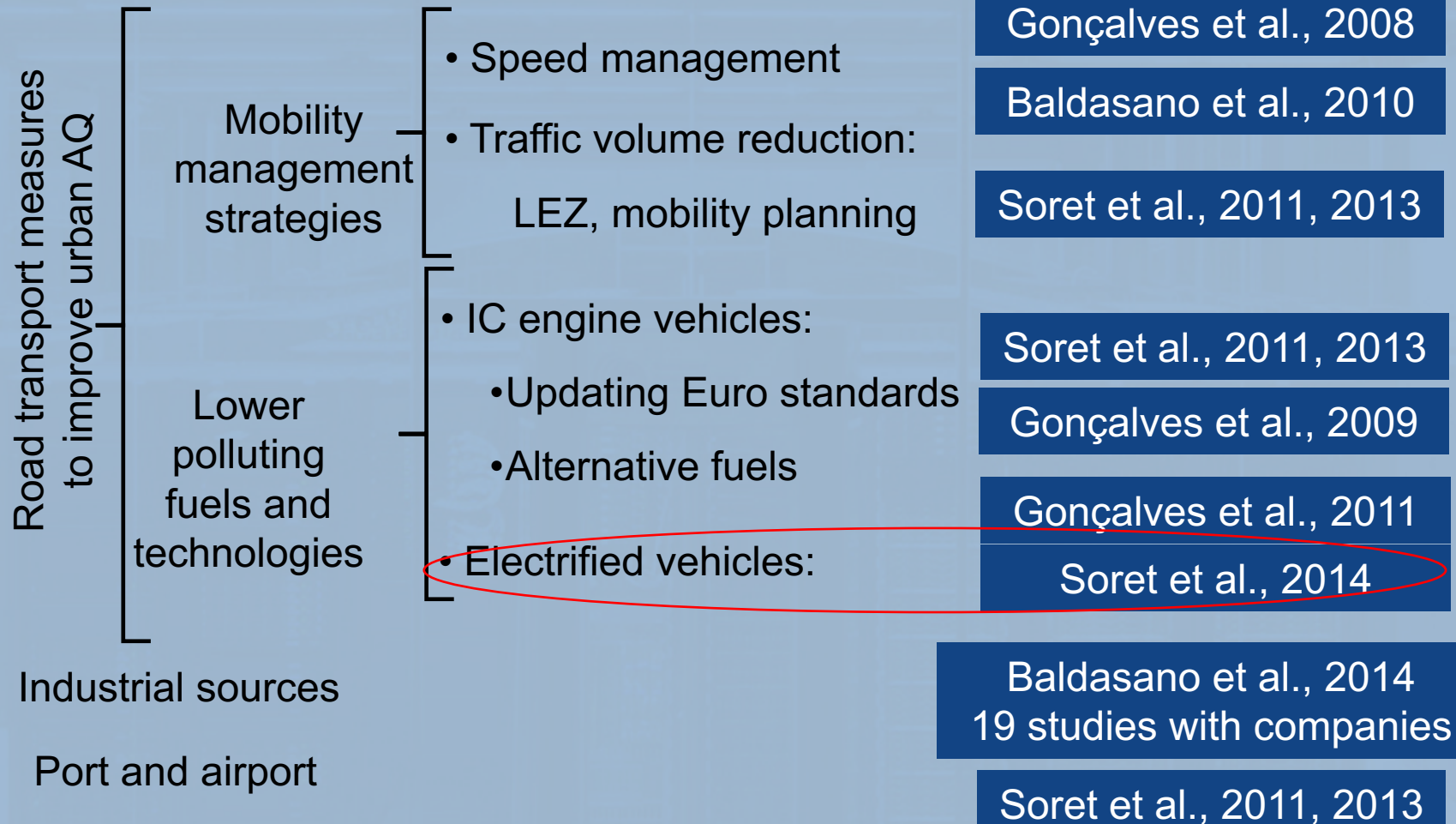


North Africa-Middle East-Europe

NMMB/BSC-Dust Dust Load ( $\text{g}/\text{m}^2$ ) and 700 hPa Wind  
36h forecast for 00UTC 02 Aug 2016










## Air quality planning





Fleet electrification: Replacement of internal combustion vehicles by electric vehicles

	Fuel red.	Autonomy	
<b>Micro-hybrid</b>	5-10%		
<b>Mild-hybrid</b>	10-20%		
<b>Full-Hybrid (HEV)</b>	20-30%	2 km	
<b>PHEV</b>	35-85%	20-80 km	
<b>Range Extender</b>	65-100%	50-120 km	
<b>BEV</b>	100%	80-300 km	
<b>Fuel cell vehicle (FCEV)</b>	H2	400-600 km	

Hybrid electric vehicles (HEV)



e.g. Van Hool Exquicity

Plug-in electric vehicle (PHEV)



e.g. Piaggio MP3 Hybrid 300

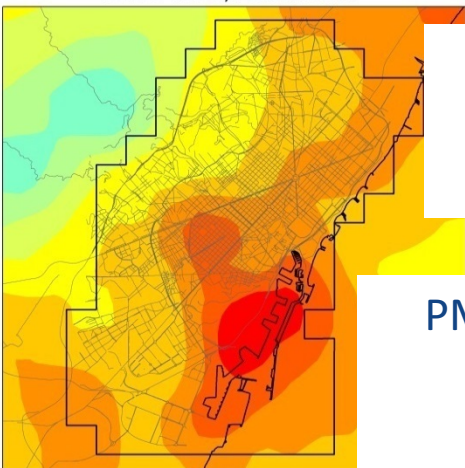
Battery electric vehicle (BEV)



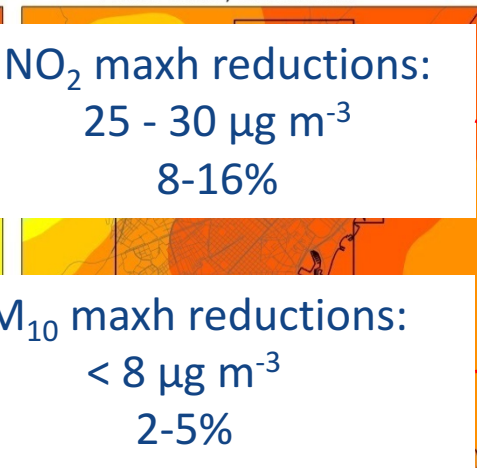
e.g. BMW i3

# Fleet electrification. Air quality impacts

NO<sub>2</sub> (ug m<sup>-3</sup>) Max h  
Base case; Barcelona



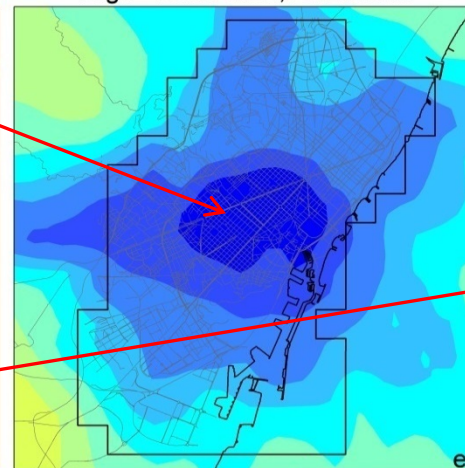
PM<sub>10</sub> (ug m<sup>-3</sup>) Max h  
Base case; Barcelona



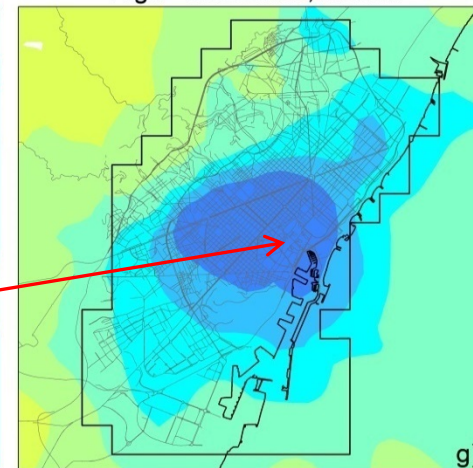
NO<sub>2</sub> maxh reductions:  
25 - 30  $\mu\text{g m}^{-3}$   
8-16%

PM<sub>10</sub> maxh reductions:  
< 8  $\mu\text{g m}^{-3}$   
2-5%

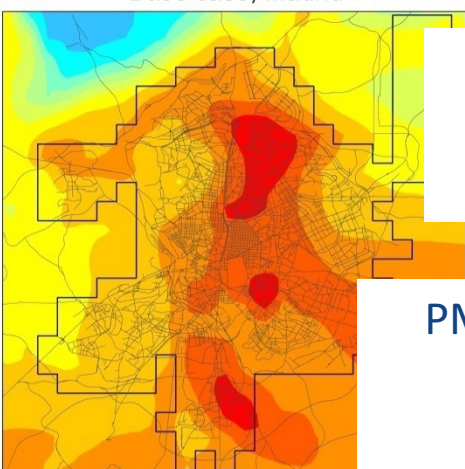
NO<sub>2</sub> (ug m<sup>-3</sup>) Max diff h  
High - Base case; Barcelona



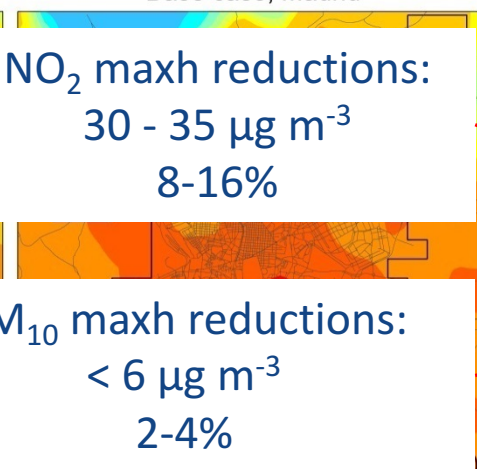
PM<sub>10</sub> (ug m<sup>-3</sup>) Max diff h  
High - Base case; Madrid



NO<sub>2</sub> (ug m<sup>-3</sup>) Max h  
Base case; Madrid



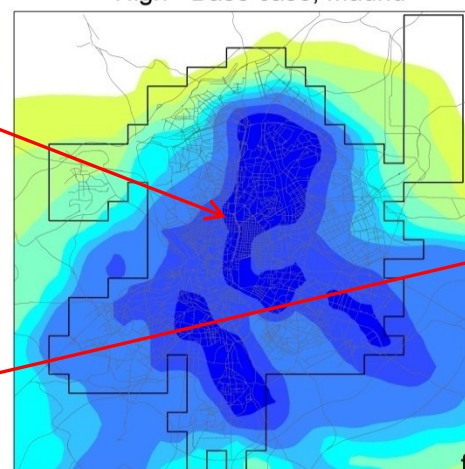
PM<sub>10</sub> (ug m<sup>-3</sup>) Max h  
Base case; Madrid



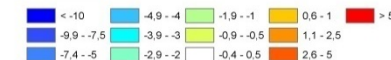
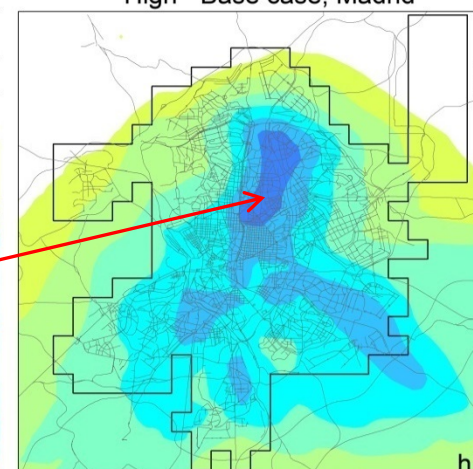
NO<sub>2</sub> maxh reductions:  
30 - 35  $\mu\text{g m}^{-3}$   
8-16%

PM<sub>10</sub> maxh reductions:  
< 6  $\mu\text{g m}^{-3}$   
2-4%

NO<sub>2</sub> (ug m<sup>-3</sup>) Max diff h  
High - Base case; Madrid



PM<sub>10</sub> (ug m<sup>-3</sup>) Max diff h  
High - Base case; Madrid





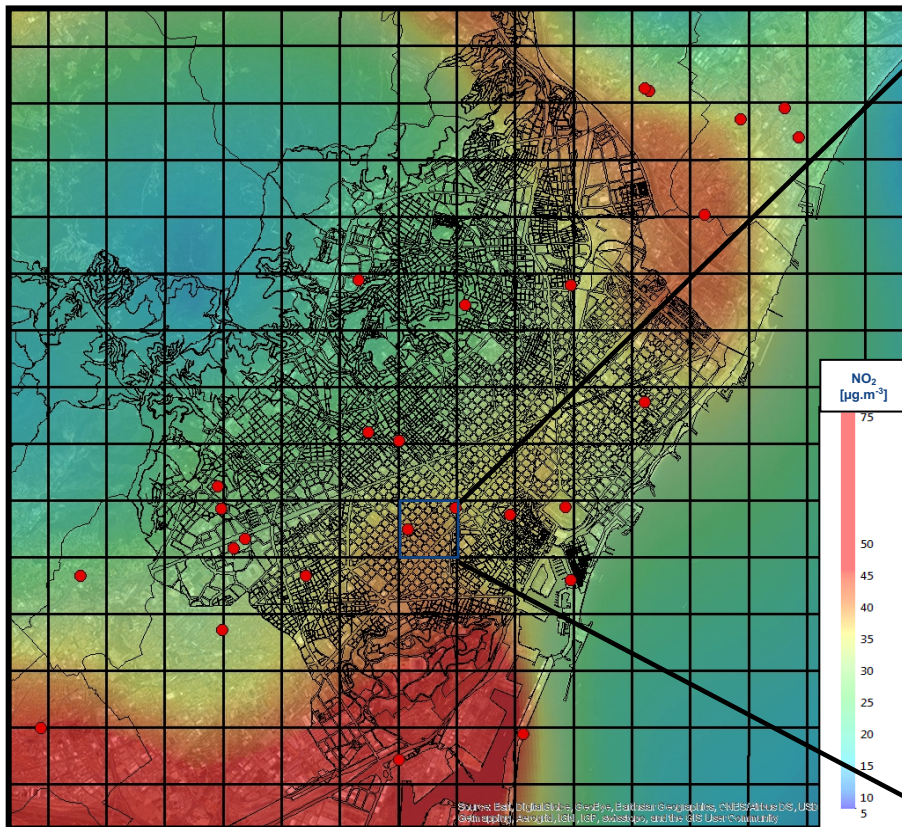
# Future work. Urban air quality modelling

PhD Jaime Benavides and PhD Daniel Rodriguez

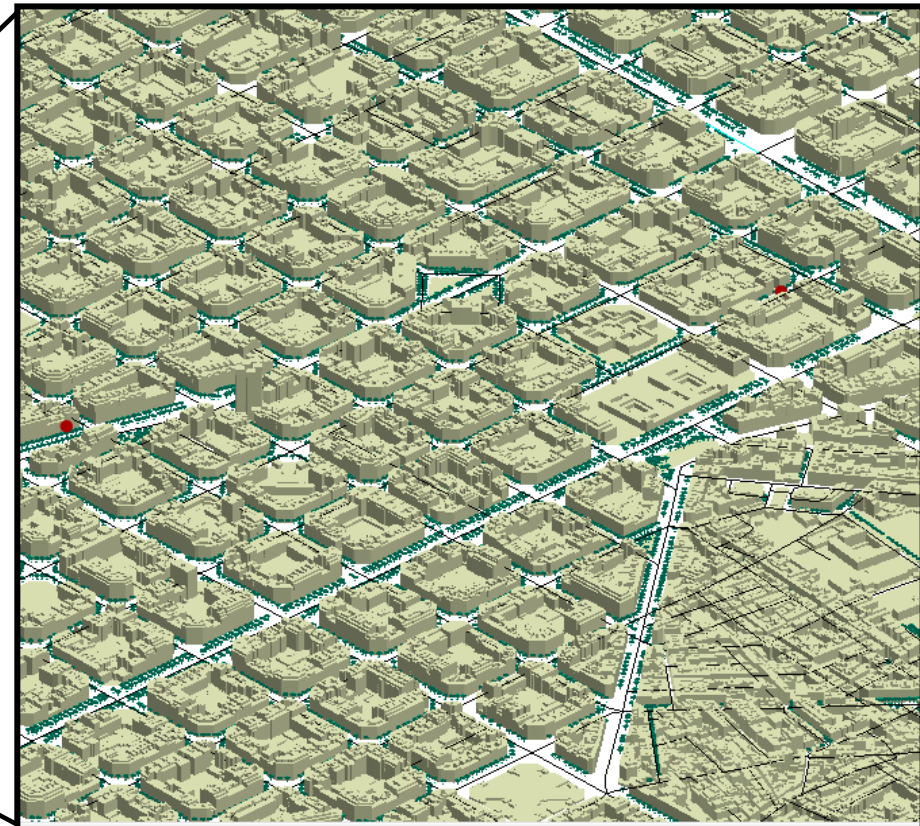




## Where we are now



# Where we want to go

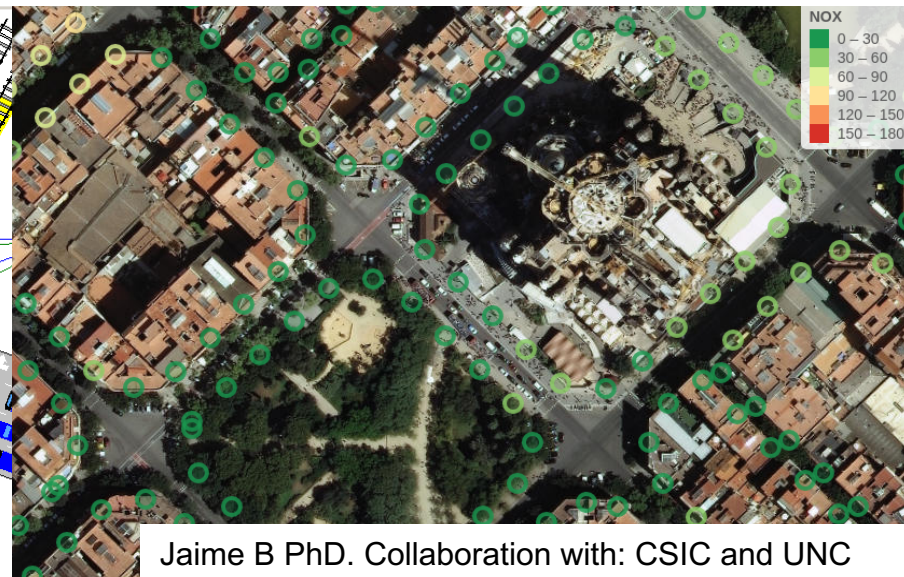
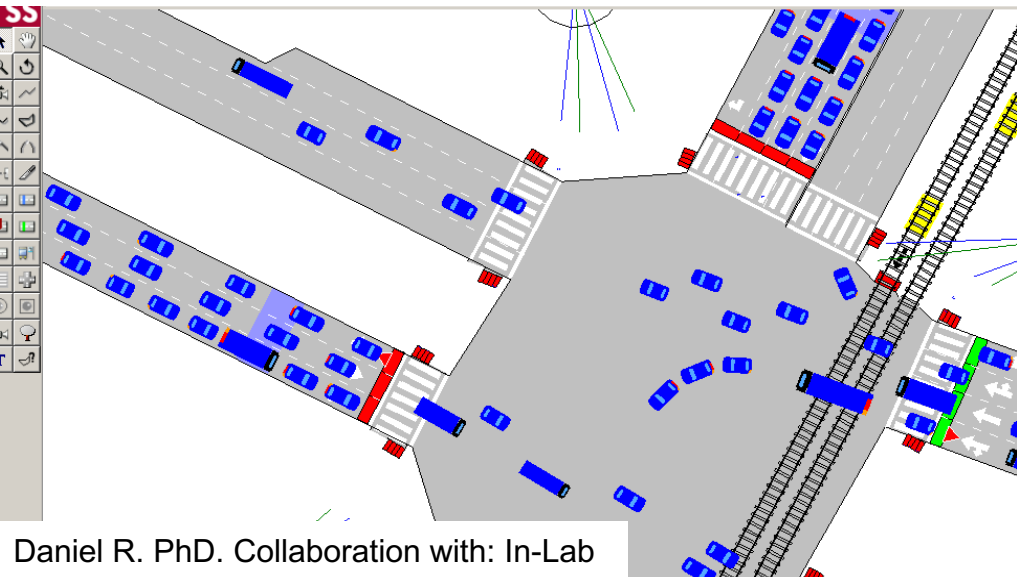
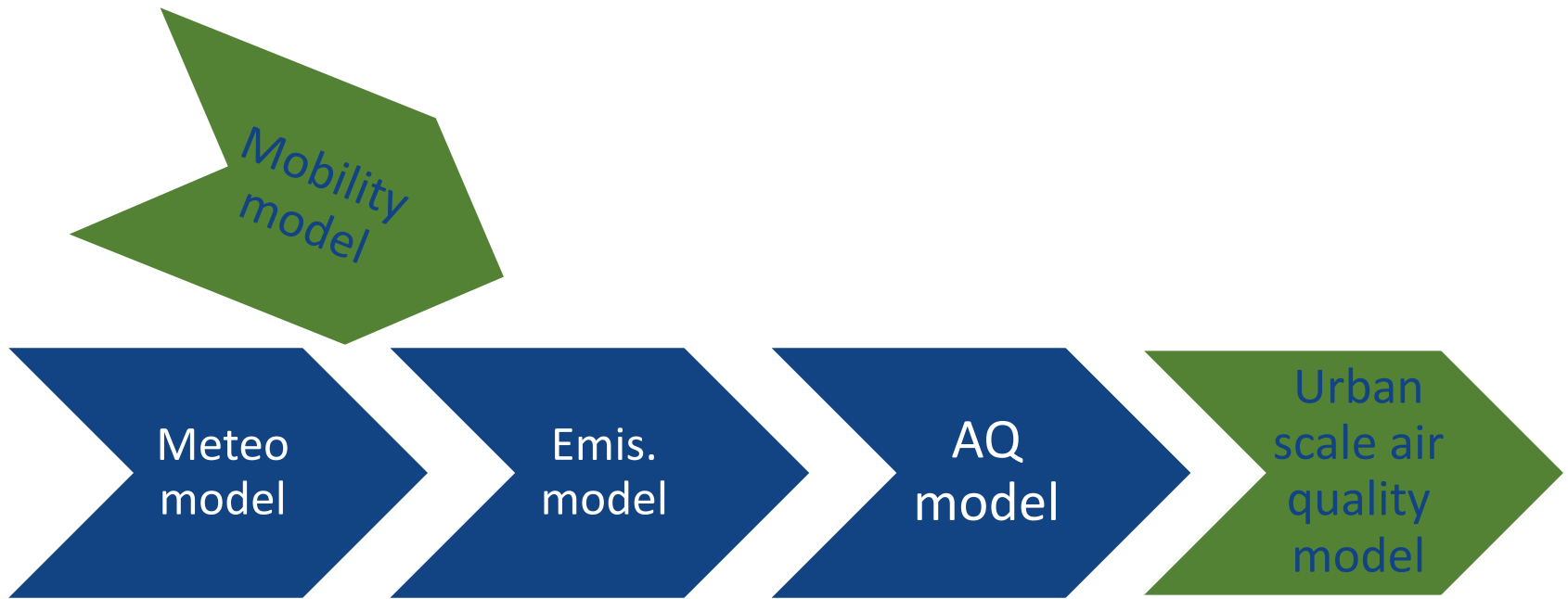




# Model chain. Two complementary PhDs



**Barcelona  
Supercomputing  
Center**  
Centro Nacional de Supercomputación



Daniel R. PhD. Collaboration with: In-Lab

Jaime B PhD. Collaboration with: CSIC and UNC

# National and International collaborations



**Barcelona  
Supercomputing  
Center**  
Centro Nacional de Supercomputación

EXCELENCIA  
SEVERO  
OCHOA

## Research centers



## Local administrations and international organizations



## Meteorological offices



Agencia Estatal de Meteorología



# National and International collaborations



**Barcelona  
Supercomputing  
Center**  
Centro Nacional de Supercomputación



## Industrial partners. Air quality

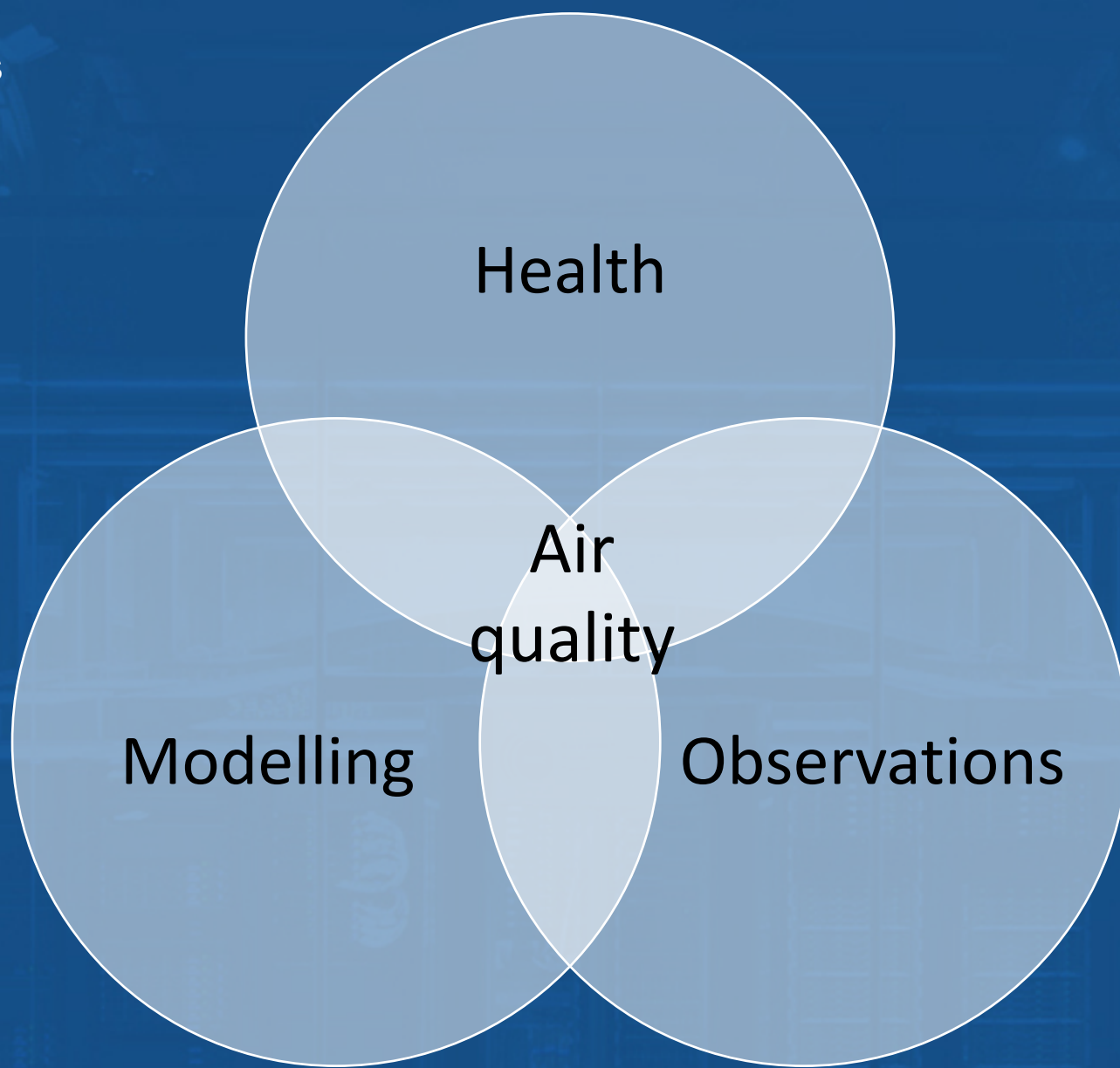


## Industrial partners. Energy



## Industrial partners. Agriculture





For further information please contact:  
carlos.perez@bsc.es, maria.pay@bsc.es and  
albert.soret@bsc.es

